Full wwPDB EM Validation Report

Jun 15, 2026 – 07:40 PM EDT

PDB ID	:	9Q3K / pdb_00009q3k
EMDB ID	:	EMD-72200
Title	:	Structure of LarA-like nickel-pincer nucleotide cofactor-utilizing enzyme with a single catalytic histidine residue from Streptococcus plurextorum
Authors	:	Subramanian, S.; Gatreddi, S.; Hausinger, R.P.; Hu, J.; Parent, K.N.
Deposited on	:	2025-08-18
Resolution	:	2.20 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

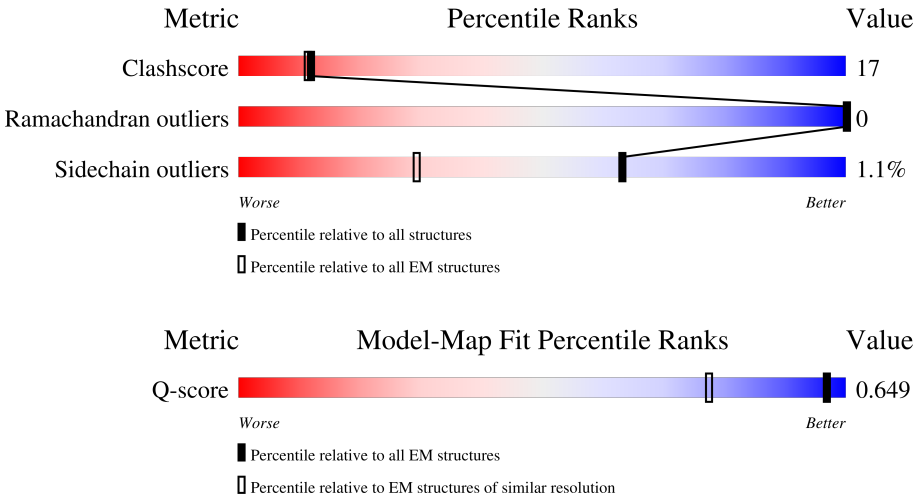
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	3184 (1.71 - 2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	498	10% 62% 34%
1	B	498	9% 60% 36%
1	C	498	10% 61% 35%
1	D	498	10% 62% 34%

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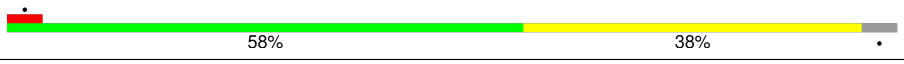
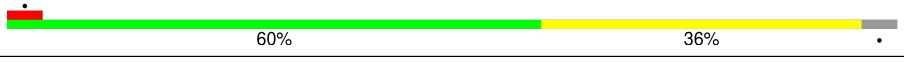
Mol	Chain	Length	Quality of chain
1	E	498	
1	F	498	
1	G	498	
1	H	498	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	4EY	F	502	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 30332 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called LarA-like nickel-pincer nucleotide cofactor-utilizing enzyme.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	480	Total 3753	C 2395	N 635	O 697	S 26	0	0
1	D	480	Total 3762	C 2401	N 634	O 700	S 27	1	0
1	A	480	Total 3764	C 2403	N 635	O 699	S 27	1	0
1	H	480	Total 3772	C 2408	N 638	O 700	S 26	0	0
1	E	480	Total 3772	C 2407	N 638	O 700	S 27	1	0
1	F	480	Total 3772	C 2408	N 638	O 700	S 26	0	0
1	C	480	Total 3764	C 2403	N 635	O 699	S 27	1	0
1	G	480	Total 3773	C 2410	N 638	O 698	S 27	1	0

- Molecule 2 is NICKEL (II) ION (CCD ID: NI) (formula: Ni) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
2	B	1	Total 1	Ni 1	0
2	D	1	Total 1	Ni 1	0
2	A	1	Total 1	Ni 1	0
2	H	1	Total 1	Ni 1	0
2	E	1	Total 1	Ni 1	0
2	F	1	Total 1	Ni 1	0

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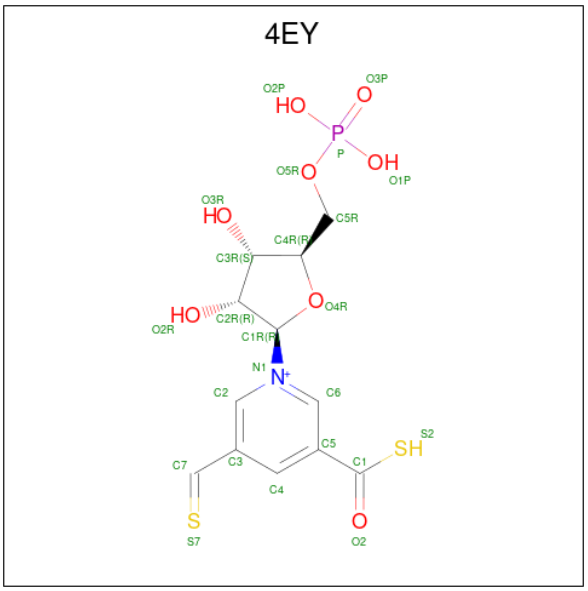
Mol	Chain	Residues	Atoms	AltConf
2	C	1	Total Ni 1 1	0
2	G	1	Total Ni 1 1	0

- Molecule 3 is 3-methanethioyl-1-(5-O-phosphono-beta-D-ribofuranosyl)-5-(sulfanylcarbonyl)pyridin-1-ium (CCD ID: 4EY) (formula: $C_{12}H_{15}NO_8PS_2$) (labeled as "Ligand of Interest" by depositor).



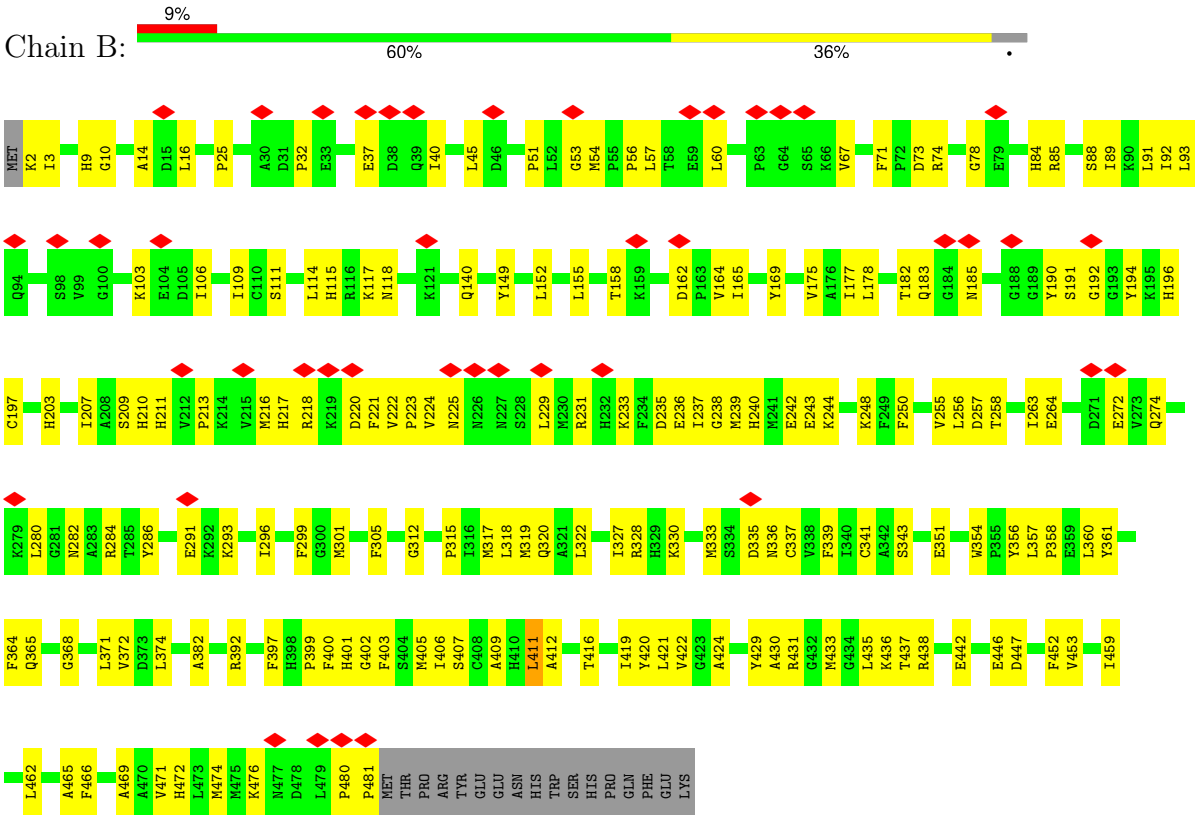
Mol	Chain	Residues	Atoms	AltConf
3	B	1	Total C N O P S 24 12 1 8 1 2	0
3	D	1	Total C N O P S 24 12 1 8 1 2	0
3	A	1	Total C N O P S 24 12 1 8 1 2	0
3	H	1	Total C N O P S 24 12 1 8 1 2	0
3	E	1	Total C N O P S 24 12 1 8 1 2	0
3	F	1	Total C N O P S 24 12 1 8 1 2	0
3	C	1	Total C N O P S 24 12 1 8 1 2	0
3	G	1	Total C N O P S 24 12 1 8 1 2	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

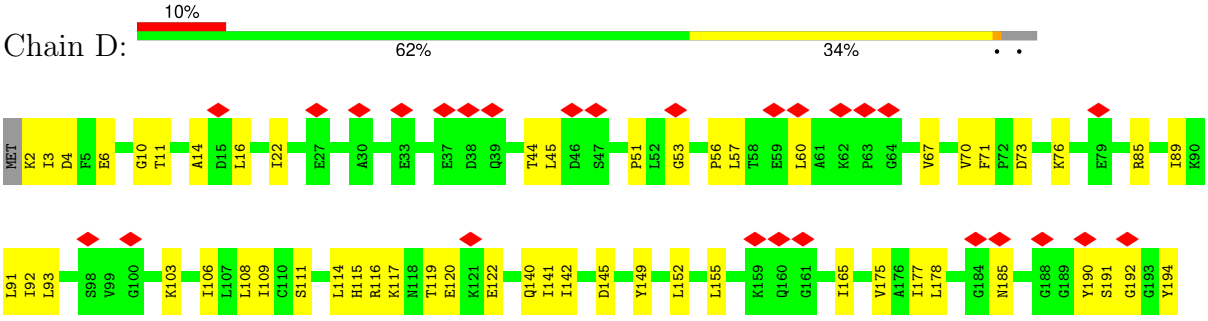
• Molecule 1: LarA-like nickel-pincer nucleotide cofactor-utilizing enzyme

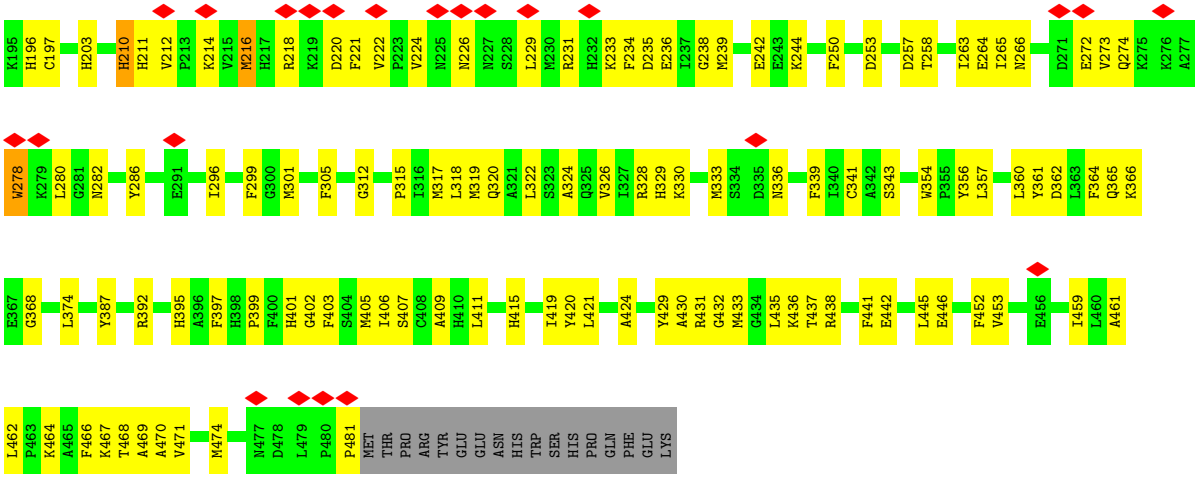
Chain B:



• Molecule 1: LarA-like nickel-pincer nucleotide cofactor-utilizing enzyme

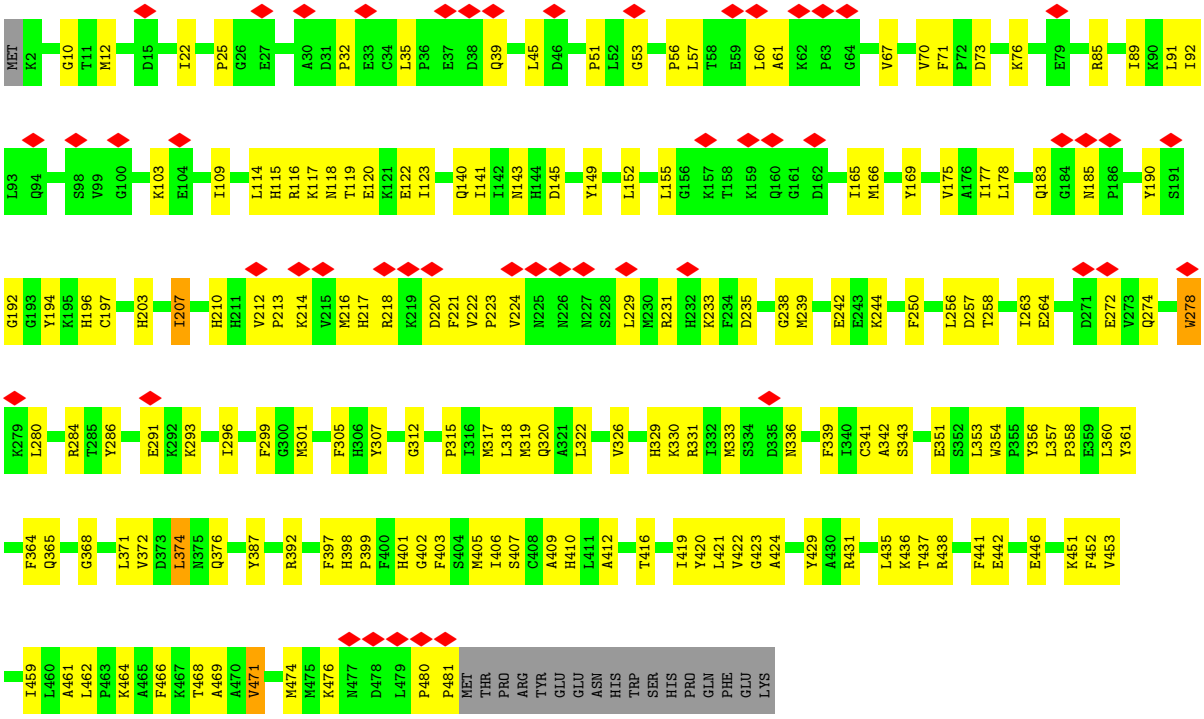
Chain D:





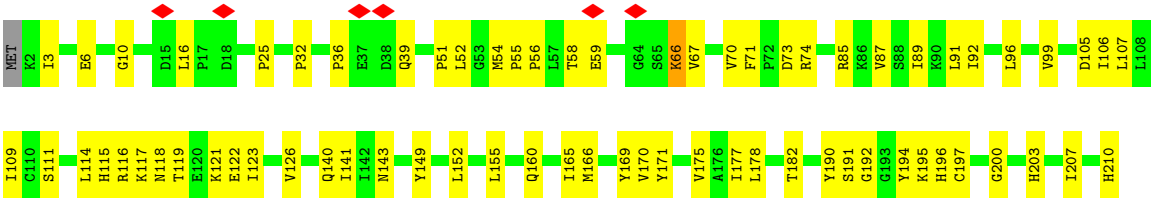
• Molecule 1: LarA-like nickel-pincer nucleotide cofactor-utilizing enzyme

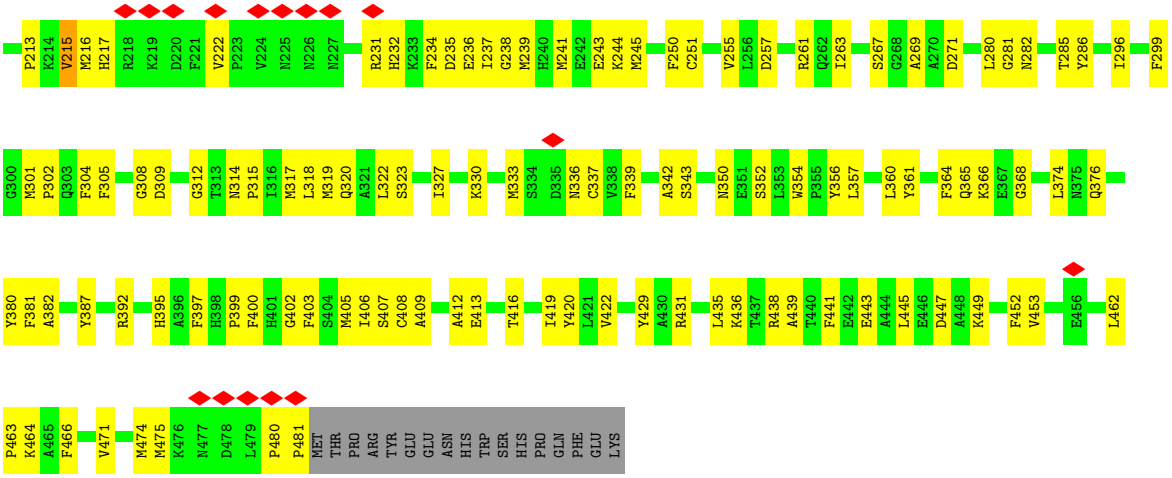
Chain A:



• Molecule 1: LarA-like nickel-pincer nucleotide cofactor-utilizing enzyme

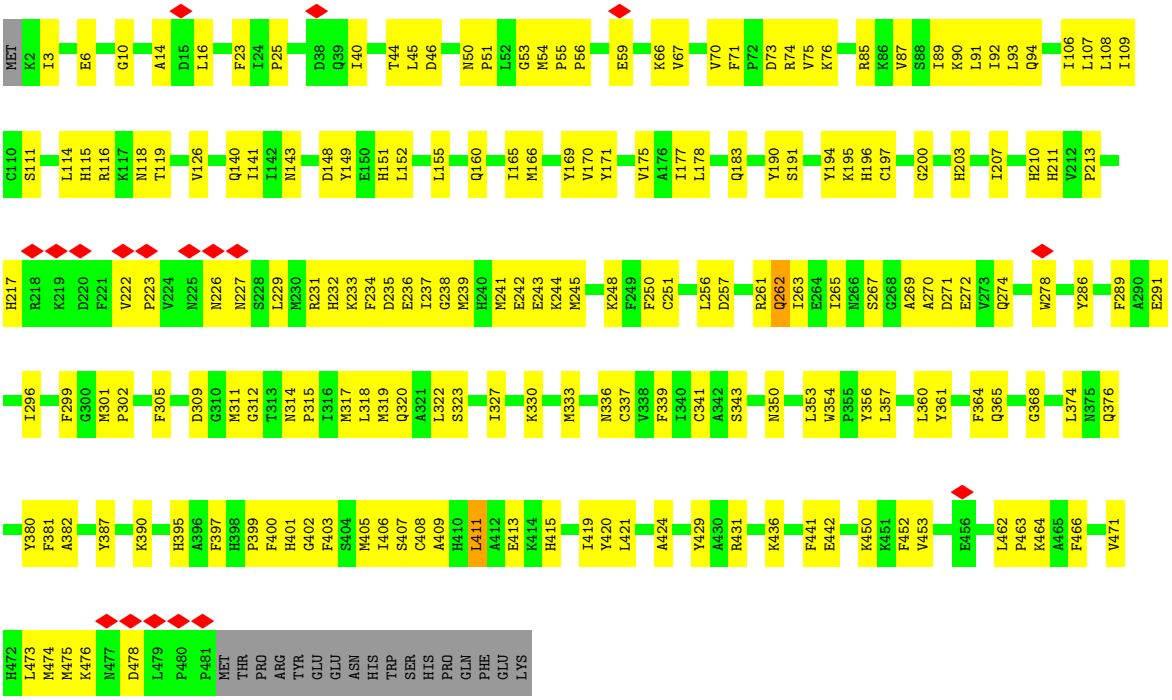
Chain H:





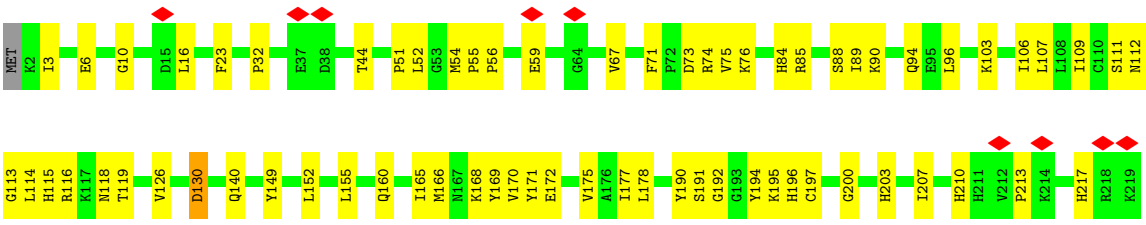
• Molecule 1: LarA-like nickel-pincer nucleotide cofactor-utilizing enzyme

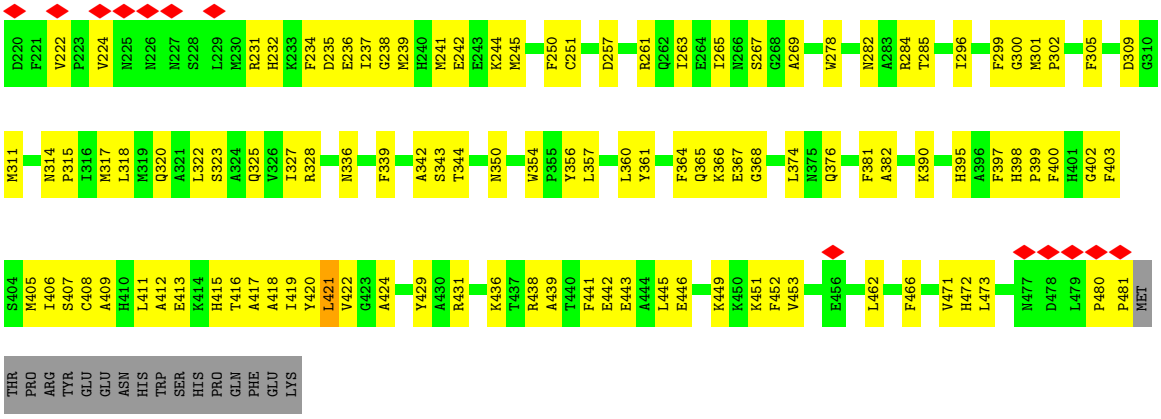
Chain E:



• Molecule 1: LarA-like nickel-pincer nucleotide cofactor-utilizing enzyme

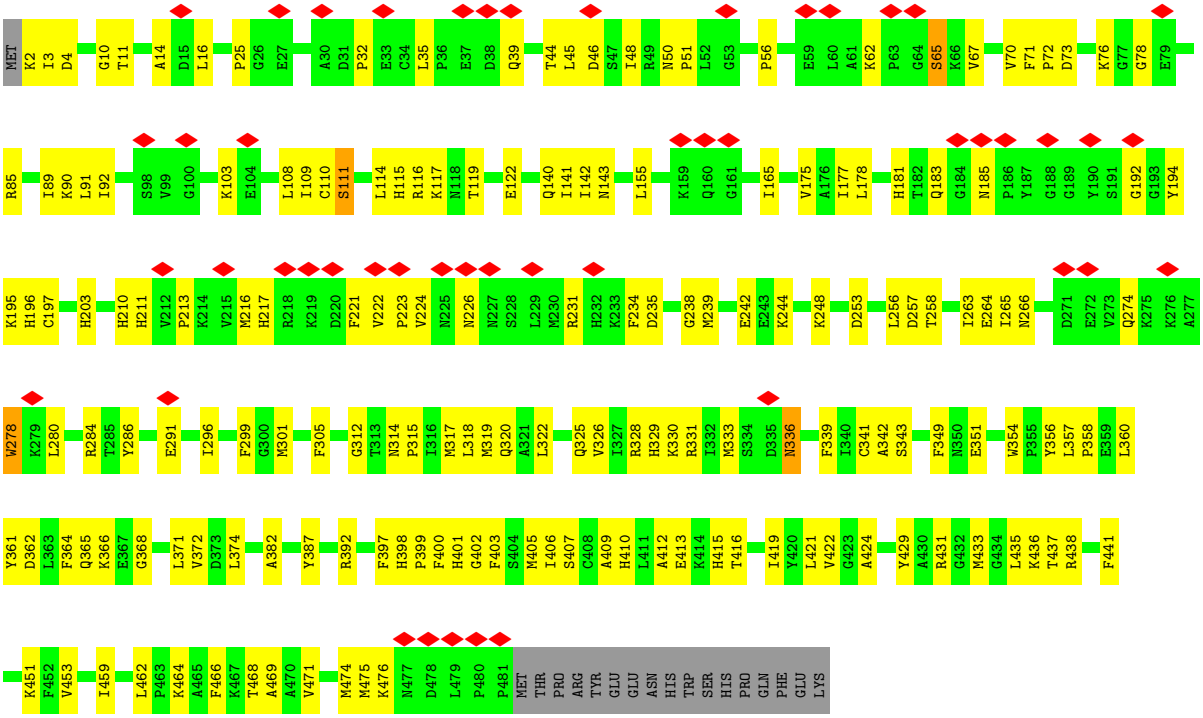
Chain F:





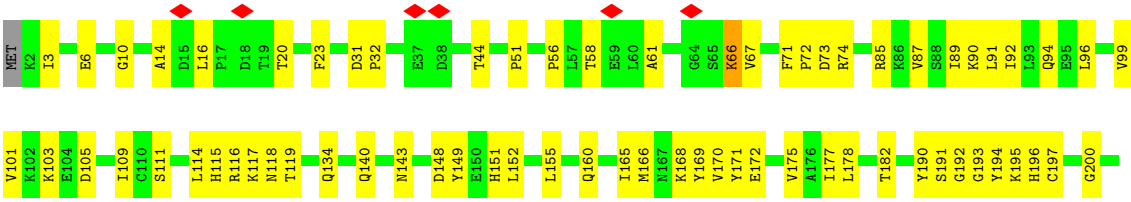
• Molecule 1: LarA-like nickel-pincer nucleotide cofactor-utilizing enzyme

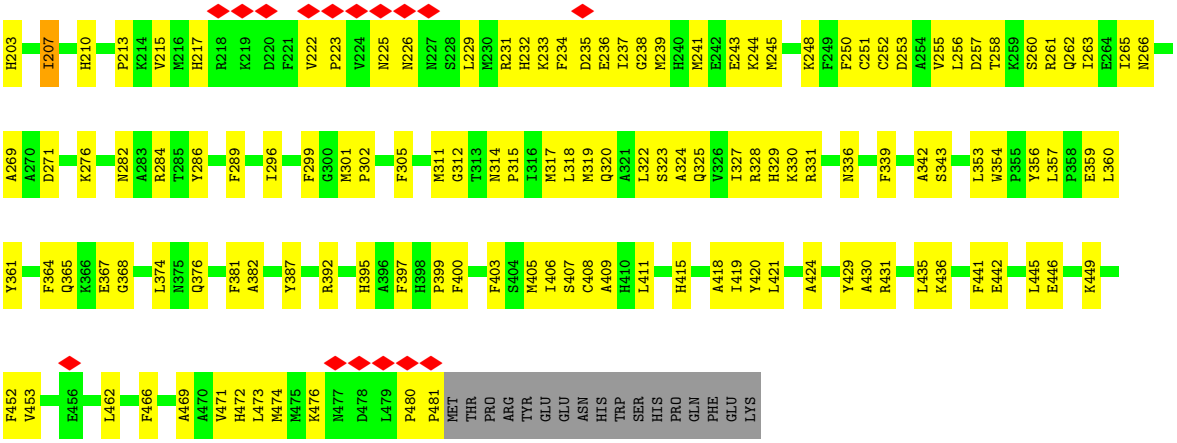
Chain C:



• Molecule 1: LarA-like nickel-pincer nucleotide cofactor-utilizing enzyme

Chain G:




H203 I207 H210 P213 K214 V215 M216 H217 R218 K219 D220 F221 V222 P223 V224 N225 N226 N227 S228 L229 M230 R231 H232 K233 F234 D235 E236 I237 G238 M239 H240 M241 E242 E243 K244 M245 K248 F249 F250 C251 C252 D253 A254 V255 L256 D257 T258 K259 S260 R261 Q262 I263 E264 I265 N266
A269 A270 D271 K276 N282 A283 R284 T285 Y286 F289 I296 F299 G300 M301 P302 F305 M311 G312 T313 N314 P315 I316 M317 L318 M319 Q320 A321 L322 S323 A324 Q325 V326 I327 R328 H329 K330 R331 N336 F339 A342 S343 L353 W354 P355 Y356 L357 P358 E359 L360
Y361 F364 Q365 K366 E367 G368 L374 N375 Q376 F381 A382 Y387 R392 H395 A396 F397 H398 P399 F400 F403 S404 M405 I406 S407 C408 A409 H410 L411 H415 A418 I419 Y420 L421 A424 Y429 A430 R431 L435 K436 F441 E442 L445 E446 K449
F452 V453 E456 L462 F466 A469 A470 V471 H472 L473 M474 M475 K476 N477 D478 L479 P480 P481 MET THR PRO ARG TYR GLU GLU ASN HIS TRP SER HIS PRO GLN PHE GLU LYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	571000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	44.71	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	130000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.064	Depositor
Minimum map value	-0.726	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.033	Depositor
Recommended contour level	0.11	Depositor
Map size (Å)	265.8, 265.8, 265.8	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.886, 0.886, 0.886	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NI, 4EY

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.13	0/3864	0.31	0/5233
1	B	0.12	0/3848	0.29	0/5209
1	C	0.13	0/3864	0.31	0/5233
1	D	0.12	0/3861	0.30	0/5229
1	E	0.13	0/3872	0.32	0/5241
1	F	0.13	0/3869	0.32	0/5237
1	G	0.13	0/3873	0.33	0/5242
1	H	0.12	0/3869	0.31	0/5237
All	All	0.13	0/30920	0.31	0/41861

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3764	0	3656	130	0
1	B	3753	0	3652	125	0
1	C	3764	0	3656	130	0
1	D	3762	0	3655	119	0
1	E	3772	0	3673	148	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3772	0	3677	135	0
1	G	3773	0	3682	149	0
1	H	3772	0	3677	129	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	24	0	12	4	0
3	B	24	0	12	3	0
3	C	24	0	12	5	0
3	D	24	0	12	5	0
3	E	24	0	12	5	0
3	F	24	0	12	7	0
3	G	24	0	12	5	0
3	H	24	0	12	6	0
All	All	30332	0	29424	1041	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

All (1041) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:364:PHE:HB2	1:H:374:LEU:HD11	1.66	0.78
1:D:364:PHE:HB2	1:D:374:LEU:HD11	1.65	0.78
1:C:364:PHE:HB2	1:C:374:LEU:HD11	1.66	0.78
1:A:10:GLY:HA3	1:E:10:GLY:HA3	1.67	0.77
1:E:364:PHE:HB2	1:E:374:LEU:HD11	1.66	0.76
1:F:165:ILE:HB	1:F:203:HIS:HB2	1.67	0.76
1:F:364:PHE:HB2	1:F:374:LEU:HD11	1.66	0.76
1:E:165:ILE:HB	1:E:203:HIS:HB2	1.67	0.75
1:D:326:VAL:HA	1:D:333:MET:HE1	1.68	0.74
1:H:165:ILE:HB	1:H:203:HIS:HB2	1.67	0.74
1:G:364:PHE:HB2	1:G:374:LEU:HD11	1.67	0.74
1:G:165:ILE:HB	1:G:203:HIS:HB2	1.69	0.74
1:C:10:GLY:HA3	1:G:10:GLY:HA3	1.68	0.74
1:C:326:VAL:HA	1:C:333:MET:HE1	1.68	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:GLU:HG3	1:A:476:LYS:HG3	1.71	0.73
1:B:364:PHE:HB2	1:B:374:LEU:HD11	1.68	0.73
1:B:10:GLY:HA3	1:F:10:GLY:HA3	1.69	0.73
1:G:115:HIS:HD1	3:G:502:4EY:H12	1.36	0.72
1:A:326:VAL:HA	1:A:333:MET:HE1	1.70	0.72
1:H:58:THR:HA	1:H:99:VAL:HG11	1.71	0.72
1:H:121:LYS:HE3	1:H:122:GLU:HG3	1.70	0.71
1:C:318:LEU:HD11	1:C:421:LEU:HD11	1.72	0.71
1:A:217:HIS:NE2	1:A:407:SER:O	2.22	0.71
1:D:10:GLY:HA3	1:H:10:GLY:HA3	1.71	0.71
1:G:111:SER:HG	1:G:196:HIS:HE2	1.39	0.70
1:E:210:HIS:HD2	1:E:211:HIS:HD1	1.39	0.70
1:C:217:HIS:NE2	1:C:407:SER:O	2.22	0.70
1:E:3:ILE:HD12	1:E:16:LEU:HD12	1.73	0.70
1:G:314:ASN:HB3	1:G:317:MET:HB2	1.73	0.70
1:B:165:ILE:HB	1:B:203:HIS:HB2	1.73	0.69
1:D:421:LEU:HD22	1:D:424:ALA:HB2	1.74	0.69
1:A:183:GLN:HG3	1:A:256:LEU:HB2	1.75	0.69
1:F:235:ASP:O	1:F:239:MET:HG2	1.93	0.69
1:H:235:ASP:O	1:H:239:MET:HG2	1.93	0.69
1:C:165:ILE:HB	1:C:203:HIS:HB2	1.72	0.69
1:C:185:ASN:ND2	3:C:502:4EY:O2P	2.26	0.69
1:E:235:ASP:O	1:E:239:MET:HG2	1.94	0.68
1:B:421:LEU:HD22	1:B:424:ALA:HB2	1.75	0.68
1:H:216:MET:SD	1:H:407:SER:OG	2.50	0.68
1:D:165:ILE:HB	1:D:203:HIS:HB2	1.75	0.68
1:E:421:LEU:HD12	1:E:424:ALA:HB2	1.75	0.68
1:B:291:GLU:HG3	1:B:476:LYS:HG3	1.75	0.68
1:F:217:HIS:NE2	1:F:407:SER:O	2.27	0.68
1:E:223:PRO:HB3	1:E:330:LYS:HB3	1.76	0.68
1:G:257:ASP:HA	1:G:284:ARG:HD3	1.77	0.67
1:F:3:ILE:HD12	1:F:16:LEU:HD12	1.75	0.67
1:F:421:LEU:HD12	1:F:424:ALA:HB2	1.77	0.67
1:G:114:LEU:HG	1:G:207:ILE:HD13	1.75	0.67
1:G:421:LEU:HD22	1:G:424:ALA:HB2	1.76	0.67
1:E:55:PRO:HB2	1:E:59:GLU:HB2	1.76	0.67
1:E:155:LEU:O	1:E:244:LYS:NZ	2.28	0.67
1:G:222:VAL:HG12	1:G:330:LYS:HG2	1.76	0.67
1:D:339:PHE:HB2	1:D:419:ILE:HG12	1.76	0.66
1:C:362:ASP:O	1:C:366:LYS:HG2	1.95	0.66
1:G:235:ASP:O	1:G:239:MET:HG2	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:155:LEU:HB3	1:D:244:LYS:HG3	1.77	0.66
1:B:217:HIS:NE2	1:B:407:SER:O	2.22	0.65
1:C:3:ILE:HD12	1:C:16:LEU:HD12	1.78	0.65
1:B:339:PHE:HB2	1:B:419:ILE:HG12	1.78	0.65
1:A:339:PHE:HB2	1:A:419:ILE:HG12	1.78	0.65
1:E:6:GLU:HG2	1:E:302:PRO:HG3	1.79	0.65
1:C:315:PRO:HG3	1:C:429:TYR:HB3	1.79	0.65
1:A:103:LYS:O	1:A:140:GLN:NE2	2.29	0.65
1:C:242:GLU:HG2	1:C:248:LYS:HA	1.77	0.65
1:G:226:ASN:ND2	1:G:481:PRO:O	2.30	0.65
1:B:242:GLU:HG2	1:B:248:LYS:HA	1.77	0.65
1:D:218:ARG:NH1	1:D:220:ASP:OD2	2.30	0.65
1:D:103:LYS:O	1:D:140:GLN:NE2	2.30	0.64
1:D:116:ARG:HH12	1:D:119:THR:HG23	1.62	0.64
1:A:421:LEU:HD22	1:A:424:ALA:HB2	1.79	0.64
1:B:103:LYS:O	1:B:140:GLN:NE2	2.31	0.64
1:D:299:PHE:HB3	1:D:462:LEU:HB2	1.78	0.64
1:E:178:LEU:HD11	1:E:197:CYS:HB3	1.79	0.64
1:D:3:ILE:HD12	1:D:16:LEU:HD12	1.79	0.64
1:A:155:LEU:HB3	1:A:244:LYS:HG3	1.80	0.64
1:H:3:ILE:HD12	1:H:16:LEU:HD12	1.78	0.64
1:C:339:PHE:HB2	1:C:419:ILE:HG12	1.78	0.64
1:A:235:ASP:O	1:A:239:MET:HG3	1.98	0.64
1:A:315:PRO:HG3	1:A:429:TYR:HB3	1.79	0.64
1:E:114:LEU:HG	1:E:207:ILE:HD13	1.80	0.63
1:F:301:MET:HE1	1:F:322:LEU:HG	1.80	0.63
1:B:155:LEU:HB3	1:B:244:LYS:HG3	1.79	0.63
1:D:258:THR:HA	1:D:469:ALA:HB3	1.80	0.63
1:G:323:SER:O	1:G:327:ILE:HG13	1.98	0.63
1:H:323:SER:O	1:H:327:ILE:HG13	1.99	0.63
1:F:155:LEU:HB3	1:F:244:LYS:HG3	1.80	0.63
1:C:421:LEU:HD22	1:C:424:ALA:HB2	1.79	0.63
1:G:155:LEU:O	1:G:244:LYS:NZ	2.32	0.63
1:A:165:ILE:HB	1:A:203:HIS:HB2	1.78	0.63
1:E:217:HIS:NE2	1:E:407:SER:O	2.22	0.63
1:B:264:GLU:HG2	1:B:280:LEU:HD12	1.81	0.63
1:G:299:PHE:HB3	1:G:462:LEU:HB2	1.80	0.63
1:E:301:MET:HE1	1:E:322:LEU:HG	1.80	0.62
1:F:314:ASN:HB3	1:F:317:MET:HB2	1.80	0.62
1:F:436:LYS:NZ	1:C:413:GLU:OE2	2.32	0.62
1:F:191:SER:HA	1:F:195:LYS:HD3	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:LEU:HD11	1:A:421:LEU:HD11	1.80	0.62
1:C:103:LYS:O	1:C:140:GLN:NE2	2.30	0.62
1:C:299:PHE:HB3	1:C:462:LEU:HB2	1.80	0.62
1:G:226:ASN:HD21	1:G:282:ASN:HD21	1.47	0.62
1:G:339:PHE:HB2	1:G:419:ILE:HG12	1.81	0.62
1:B:235:ASP:O	1:B:239:MET:HG3	2.00	0.62
1:D:190:TYR:O	1:D:231:ARG:NH2	2.31	0.62
1:E:339:PHE:HB2	1:E:419:ILE:HG12	1.81	0.62
1:F:336:ASN:ND2	1:F:452:PHE:O	2.32	0.62
1:H:301:MET:HE1	1:H:322:LEU:HG	1.81	0.62
1:G:3:ILE:HD12	1:G:16:LEU:HD12	1.82	0.62
1:G:282:ASN:ND2	1:G:481:PRO:O	2.31	0.62
1:D:235:ASP:O	1:D:239:MET:HG3	1.99	0.61
1:A:183:GLN:HG2	1:A:284:ARG:HH21	1.64	0.61
1:G:301:MET:HE1	1:G:322:LEU:HG	1.81	0.61
1:A:25:PRO:HB3	1:A:471:VAL:HG13	1.82	0.61
1:E:191:SER:HA	1:E:195:LYS:HD3	1.83	0.61
1:F:339:PHE:HB2	1:F:419:ILE:HG12	1.82	0.61
1:F:178:LEU:HD11	1:F:197:CYS:HB3	1.82	0.61
1:F:296:ILE:HD11	1:F:453:VAL:HG21	1.82	0.61
1:F:299:PHE:HB3	1:F:462:LEU:HB2	1.83	0.61
1:C:258:THR:HA	1:C:469:ALA:HB3	1.83	0.61
1:H:190:TYR:O	1:H:231:ARG:NH2	2.27	0.61
1:C:235:ASP:O	1:C:239:MET:HG3	1.99	0.61
1:D:328:ARG:HD3	1:D:470:ALA:HB1	1.82	0.61
1:H:299:PHE:HB3	1:H:462:LEU:HB2	1.82	0.60
1:D:315:PRO:HG3	1:D:429:TYR:HB3	1.81	0.60
1:H:319:MET:HG3	1:H:409:ALA:HB1	1.83	0.60
1:B:190:TYR:O	1:B:231:ARG:NH2	2.34	0.60
1:B:315:PRO:HG3	1:B:429:TYR:HB3	1.83	0.60
1:F:402:GLY:O	1:F:405:MET:HB2	2.01	0.60
1:F:282:ASN:HB3	1:F:480:PRO:HB2	1.83	0.60
1:B:114:LEU:HG	1:B:207:ILE:HD13	1.83	0.60
1:D:360:LEU:HD21	1:D:406:ILE:HD13	1.82	0.60
1:G:111:SER:HB2	1:G:200:GLY:HA3	1.83	0.60
1:G:213:PRO:HD3	1:G:407:SER:HB2	1.83	0.59
1:G:190:TYR:O	1:G:231:ARG:NH2	2.32	0.59
1:A:57:LEU:HA	1:A:60:LEU:HD12	1.82	0.59
1:A:364:PHE:HB2	1:A:374:LEU:HD21	1.84	0.59
1:E:380:TYR:OH	1:F:390:LYS:NZ	2.35	0.59
1:C:109:ILE:HD13	1:C:142:ILE:HD11	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:67:VAL:HG22	1:C:175:VAL:HB	1.84	0.59
1:G:191:SER:HA	1:G:195:LYS:HD3	1.85	0.59
1:H:67:VAL:HG22	1:H:175:VAL:HB	1.85	0.59
1:E:296:ILE:HD11	1:E:453:VAL:HG21	1.84	0.59
1:B:73:ASP:O	1:B:85:ARG:NH1	2.36	0.59
1:H:25:PRO:HB3	1:H:471:VAL:HG13	1.84	0.59
1:A:114:LEU:HG	1:A:207:ILE:HD13	1.85	0.59
1:E:155:LEU:HB3	1:E:244:LYS:HG3	1.85	0.59
1:E:210:HIS:HD2	1:E:211:HIS:ND1	2.01	0.59
1:E:222:VAL:HG12	1:E:330:LYS:HG2	1.85	0.59
1:G:90:LYS:O	1:G:94:GLN:HG2	2.03	0.59
1:D:67:VAL:HG22	1:D:175:VAL:HB	1.84	0.58
1:C:312:GLY:O	1:C:343:SER:OG	2.20	0.58
1:H:296:ILE:HD11	1:H:453:VAL:HG21	1.85	0.58
1:F:232:HIS:O	1:F:236:GLU:HG3	2.03	0.58
1:G:178:LEU:HD11	1:G:197:CYS:HB3	1.85	0.58
1:D:464:LYS:HB3	1:D:468:THR:HG23	1.85	0.58
1:A:67:VAL:HG22	1:A:175:VAL:HB	1.85	0.58
1:G:73:ASP:O	1:G:85:ARG:NH1	2.36	0.58
1:B:336:ASN:ND2	1:B:452:PHE:O	2.37	0.58
1:F:343:SER:HB3	1:F:421:LEU:HD21	1.86	0.58
1:D:185:ASN:ND2	3:D:502:4EY:O2P	2.37	0.58
1:F:418:ALA:HB1	1:F:436:LYS:HD2	1.85	0.58
1:G:67:VAL:HG22	1:G:175:VAL:HB	1.85	0.58
1:A:258:THR:HA	1:A:469:ALA:HB3	1.85	0.58
1:H:54:MET:HE3	1:H:269:ALA:HA	1.86	0.58
1:F:282:ASN:ND2	1:F:481:PRO:O	2.35	0.58
1:E:190:TYR:O	1:E:231:ARG:NH2	2.36	0.58
1:F:237:ILE:O	1:F:241:MET:HG3	2.04	0.58
1:E:314:ASN:HB3	1:E:317:MET:HB2	1.84	0.57
1:A:190:TYR:O	1:A:231:ARG:NH2	2.36	0.57
1:H:155:LEU:HB3	1:H:244:LYS:HG3	1.85	0.57
1:H:380:TYR:OH	1:E:390:LYS:NZ	2.37	0.57
1:E:312:GLY:O	1:E:343:SER:OG	2.20	0.57
1:F:55:PRO:HB2	1:F:59:GLU:HB2	1.85	0.57
1:H:314:ASN:HB3	1:H:317:MET:HB2	1.86	0.57
1:F:320:GLN:HG2	1:F:408:CYS:HB3	1.87	0.57
1:G:217:HIS:NE2	1:G:407:SER:O	2.30	0.57
1:E:274:GLN:O	1:E:278:TRP:HB2	2.04	0.57
1:F:451:LYS:NZ	1:C:413:GLU:O	2.38	0.57
1:B:57:LEU:HA	1:B:60:LEU:HD12	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:ASN:ND2	1:B:191:SER:OG	2.35	0.57
1:H:402:GLY:O	1:H:405:MET:HB2	2.05	0.57
1:E:315:PRO:HG3	1:E:429:TYR:HB3	1.87	0.57
1:G:207:ILE:HA	1:G:210:HIS:CE1	2.39	0.57
1:B:299:PHE:HB3	1:B:462:LEU:HB2	1.85	0.57
1:C:192:GLY:HA2	1:C:196:HIS:HB2	1.86	0.57
1:A:116:ARG:HH12	1:A:119:THR:HG23	1.70	0.57
1:F:207:ILE:HA	1:F:210:HIS:CE1	2.40	0.57
1:D:238:GLY:O	1:D:242:GLU:HG2	2.05	0.57
1:B:312:GLY:O	1:B:343:SER:OG	2.23	0.56
1:H:73:ASP:OD2	3:H:502:4EY:O2R	2.20	0.56
1:E:74:ARG:H	1:E:118:ASN:HD21	1.52	0.56
1:G:237:ILE:O	1:G:241:MET:HG3	2.05	0.56
1:A:73:ASP:O	1:A:85:ARG:NH1	2.38	0.56
1:A:360:LEU:HD21	1:A:406:ILE:HD13	1.87	0.56
1:E:239:MET:O	1:E:243:GLU:HG2	2.05	0.56
1:H:315:PRO:HG3	1:H:429:TYR:HB3	1.88	0.56
1:B:360:LEU:HD21	1:B:406:ILE:HD13	1.87	0.56
1:F:32:PRO:HB2	1:F:263:ILE:HG21	1.88	0.56
1:B:192:GLY:HA2	1:B:196:HIS:HB2	1.88	0.56
1:H:74:ARG:H	1:H:118:ASN:HD21	1.53	0.56
1:D:312:GLY:O	1:D:343:SER:OG	2.24	0.56
1:E:106:ILE:O	1:E:140:GLN:NE2	2.39	0.56
1:G:324:ALA:O	1:G:328:ARG:HG3	2.06	0.56
1:G:58:THR:HA	1:G:99:VAL:HG11	1.87	0.56
1:G:315:PRO:HG3	1:G:429:TYR:HB3	1.87	0.56
1:E:67:VAL:HG22	1:E:175:VAL:HB	1.88	0.55
1:E:115:HIS:ND1	3:E:502:4EY:O2R	2.38	0.55
1:G:320:GLN:HG2	1:G:408:CYS:HB3	1.87	0.55
1:G:223:PRO:HB3	1:G:330:LYS:HB3	1.87	0.55
1:B:222:VAL:HG12	1:B:330:LYS:HG2	1.87	0.55
1:E:46:ASP:OD1	1:E:50:ASN:ND2	2.39	0.55
1:E:237:ILE:O	1:E:241:MET:HG3	2.06	0.55
1:A:207:ILE:HA	1:A:210:HIS:CE1	2.42	0.55
1:E:403:PHE:HA	1:E:406:ILE:HG12	1.88	0.55
1:F:171:TYR:CD2	1:F:245:MET:HG2	2.42	0.55
1:G:222:VAL:HG21	1:G:411:LEU:HG	1.87	0.55
1:A:192:GLY:HA2	1:A:196:HIS:HB2	1.89	0.55
1:E:46:ASP:O	1:E:50:ASN:ND2	2.39	0.55
1:F:76:LYS:O	1:F:85:ARG:NH1	2.38	0.55
1:F:315:PRO:HG3	1:F:429:TYR:HB3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:73:ASP:O	1:C:85:ARG:NH1	2.40	0.55
1:H:360:LEU:HD21	1:H:406:ILE:HD13	1.88	0.55
1:E:299:PHE:HB3	1:E:462:LEU:HB2	1.89	0.55
1:E:323:SER:O	1:E:327:ILE:HG13	2.06	0.55
1:C:360:LEU:HD21	1:C:406:ILE:HD13	1.89	0.55
1:B:210:HIS:HD2	1:B:211:HIS:HD1	1.53	0.55
1:A:299:PHE:HB3	1:A:462:LEU:HB2	1.88	0.55
1:A:301:MET:HE1	1:A:322:LEU:HG	1.89	0.55
1:E:195:LYS:HB2	1:E:231:ARG:HH12	1.72	0.55
1:F:67:VAL:HG22	1:F:175:VAL:HB	1.88	0.55
1:G:241:MET:O	1:G:245:MET:HG3	2.06	0.55
1:H:6:GLU:HG2	1:H:302:PRO:HG3	1.88	0.55
1:F:177:ILE:HG23	1:F:250:PHE:HD2	1.72	0.55
1:G:155:LEU:HB3	1:G:244:LYS:HG3	1.89	0.55
1:E:76:LYS:O	1:E:85:ARG:NH1	2.38	0.55
1:G:257:ASP:HB3	1:G:263:ILE:HD11	1.89	0.55
1:A:178:LEU:HD11	1:A:197:CYS:HB3	1.89	0.54
1:F:406:ILE:HA	1:F:409:ALA:HB3	1.89	0.54
1:A:264:GLU:HG2	1:A:280:LEU:HD12	1.88	0.54
1:F:73:ASP:O	1:F:85:ARG:NH1	2.41	0.54
1:C:361:TYR:O	1:C:365:GLN:HG2	2.07	0.54
1:B:183:GLN:HG2	1:B:284:ARG:HH21	1.72	0.54
1:H:237:ILE:O	1:H:241:MET:HG3	2.08	0.54
1:H:339:PHE:HB2	1:H:419:ILE:HG12	1.89	0.54
1:D:192:GLY:HA2	1:D:196:HIS:HB2	1.88	0.54
1:A:229:LEU:O	1:A:233:LYS:HG2	2.07	0.54
1:A:336:ASN:ND2	1:A:452:PHE:O	2.40	0.54
1:E:241:MET:O	1:E:245:MET:HG3	2.08	0.54
1:C:264:GLU:HG2	1:C:280:LEU:HD12	1.88	0.54
1:A:73:ASP:OD2	3:A:502:4EY:O2R	2.26	0.54
1:D:387:TYR:HB3	1:D:399:PRO:HG3	1.90	0.54
1:H:73:ASP:O	1:H:85:ARG:NH1	2.41	0.54
1:E:402:GLY:O	1:E:405:MET:HB2	2.06	0.54
1:E:25:PRO:HB3	1:E:471:VAL:HG13	1.88	0.54
1:E:54:MET:HE3	1:E:269:ALA:HA	1.90	0.54
3:C:502:4EY:O1P	3:C:502:4EY:H11	2.08	0.54
1:G:74:ARG:H	1:G:118:ASN:HD21	1.53	0.54
1:B:229:LEU:O	1:B:233:LYS:HG2	2.07	0.54
1:E:322:LEU:HD13	1:E:419:ILE:HG21	1.90	0.54
1:B:111:SER:O	3:B:502:4EY:O3R	2.22	0.54
1:A:76:LYS:O	1:A:85:ARG:NH1	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:109:ILE:HD11	1:H:169:TYR:HB2	1.88	0.53
1:A:257:ASP:HB3	1:A:263:ILE:HD11	1.89	0.53
1:H:191:SER:HA	1:H:195:LYS:HD3	1.90	0.53
1:E:177:ILE:HG23	1:E:250:PHE:HD2	1.73	0.53
1:H:192:GLY:HA2	1:H:196:HIS:HB2	1.90	0.53
1:B:301:MET:HE1	1:B:322:LEU:HG	1.90	0.53
1:A:212:VAL:HG22	1:A:214:LYS:H	1.73	0.53
1:H:111:SER:HB2	1:H:200:GLY:HA3	1.90	0.53
1:E:171:TYR:CD2	1:E:245:MET:HG2	2.43	0.53
1:F:74:ARG:H	1:F:118:ASN:HD21	1.55	0.53
1:C:35:LEU:HD22	1:C:39:GLN:HG2	1.91	0.53
1:B:25:PRO:HB3	1:B:471:VAL:HG13	1.90	0.53
1:B:258:THR:HA	1:B:469:ALA:HB3	1.89	0.53
1:F:368:GLY:O	1:C:431:ARG:NH1	2.36	0.53
1:C:405:MET:O	1:C:409:ALA:N	2.39	0.53
1:G:182:THR:HB	1:G:255:VAL:HG22	1.90	0.53
1:G:257:ASP:OD1	1:G:261:ARG:N	2.37	0.53
1:B:178:LEU:HD11	1:B:197:CYS:HB3	1.91	0.53
1:B:403:PHE:O	1:B:406:ILE:HG12	2.09	0.53
1:B:3:ILE:HD12	1:B:16:LEU:HD12	1.91	0.53
1:A:296:ILE:HD11	1:A:453:VAL:HG21	1.90	0.53
1:D:92:ILE:HD13	1:D:177:ILE:HG21	1.92	0.52
1:D:93:LEU:HD21	1:D:106:ILE:HG21	1.91	0.52
1:A:319:MET:SD	1:A:435:LEU:HD21	2.50	0.52
1:E:361:TYR:O	1:E:365:GLN:HG2	2.09	0.52
1:D:431:ARG:NH1	1:G:368:GLY:O	2.38	0.52
1:H:171:TYR:CD1	1:H:245:MET:HG2	2.44	0.52
1:H:222:VAL:HG12	1:H:330:LYS:HG3	1.91	0.52
1:E:51:PRO:HG3	1:E:56:PRO:HA	1.91	0.52
1:G:258:THR:HA	1:G:469:ALA:HB3	1.91	0.52
1:G:171:TYR:CD2	1:G:245:MET:HG2	2.44	0.52
1:G:319:MET:HG3	1:G:409:ALA:HB1	1.91	0.52
1:H:106:ILE:O	1:H:140:GLN:NE2	2.41	0.52
1:B:71:PHE:HB3	1:B:89:ILE:HD11	1.91	0.52
1:H:207:ILE:HA	1:H:210:HIS:CE1	2.45	0.52
1:F:54:MET:HE3	1:F:269:ALA:HA	1.92	0.52
1:C:296:ILE:HD11	1:C:453:VAL:HG21	1.91	0.52
1:G:6:GLU:HG2	1:G:302:PRO:HG3	1.91	0.52
1:G:103:LYS:O	1:G:140:GLN:NE2	2.32	0.52
1:A:223:PRO:HG3	1:A:331:ARG:HG3	1.90	0.52
1:H:178:LEU:HD11	1:H:197:CYS:HB3	1.89	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:406:ILE:HA	1:E:409:ALA:HB3	1.92	0.52
1:F:51:PRO:HG3	1:F:56:PRO:HA	1.92	0.52
1:F:241:MET:O	1:F:245:MET:HG3	2.09	0.52
1:C:387:TYR:HB3	1:C:399:PRO:HG3	1.91	0.52
1:G:111:SER:O	3:G:502:4EY:O3R	2.27	0.52
1:D:73:ASP:O	1:D:85:ARG:NH1	2.42	0.52
1:E:92:ILE:HD13	1:E:177:ILE:HG21	1.92	0.52
1:F:109:ILE:HD11	1:F:169:TYR:HB2	1.91	0.52
1:C:222:VAL:HG11	1:C:415:HIS:NE2	2.25	0.52
1:D:229:LEU:O	1:D:233:LYS:HG2	2.10	0.52
1:D:403:PHE:O	1:D:406:ILE:HG12	2.10	0.52
1:A:312:GLY:O	1:A:343:SER:OG	2.27	0.52
1:A:436:LYS:NZ	1:H:413:GLU:OE2	2.42	0.52
1:H:111:SER:HG	1:H:196:HIS:HE2	1.56	0.52
1:F:317:MET:SD	1:F:405:MET:HG3	2.50	0.52
1:G:266:ASN:ND2	1:G:276:LYS:HG2	2.25	0.52
1:H:232:HIS:O	1:H:236:GLU:HG3	2.10	0.52
1:G:149:TYR:HA	1:G:152:LEU:HB2	1.92	0.52
1:D:437:THR:O	1:D:438:ARG:NH1	2.38	0.52
1:A:274:GLN:HG2	1:A:278:TRP:CH2	2.45	0.52
1:E:73:ASP:O	1:E:85:ARG:NH1	2.44	0.52
1:B:368:GLY:O	1:E:431:ARG:NH1	2.40	0.51
1:A:361:TYR:O	1:A:365:GLN:HG2	2.10	0.51
1:H:55:PRO:HB2	1:H:59:GLU:HB2	1.92	0.51
1:E:257:ASP:HB3	1:E:263:ILE:HD11	1.91	0.51
1:C:25:PRO:HB3	1:C:471:VAL:HG13	1.92	0.51
1:G:296:ILE:HD11	1:G:453:VAL:HG21	1.91	0.51
1:B:319:MET:SD	1:B:435:LEU:HD21	2.50	0.51
1:A:53:GLY:HA3	1:A:272:GLU:HG2	1.92	0.51
1:C:111:SER:O	3:C:502:4EY:H13	2.10	0.51
1:B:436:LYS:NZ	1:E:413:GLU:OE2	2.43	0.51
1:D:264:GLU:HG2	1:D:280:LEU:HD12	1.93	0.51
1:C:92:ILE:HD13	1:C:177:ILE:HG21	1.92	0.51
1:G:92:ILE:HD13	1:G:177:ILE:HG21	1.91	0.51
1:A:71:PHE:HB3	1:A:89:ILE:HD11	1.93	0.51
1:A:114:LEU:HB3	1:A:401:HIS:HB2	1.91	0.51
1:E:291:GLU:HG3	1:E:476:LYS:HD3	1.92	0.51
1:G:103:LYS:NZ	1:G:134:GLN:O	2.36	0.51
1:D:51:PRO:HG3	1:D:56:PRO:HA	1.93	0.51
1:D:57:LEU:HA	1:D:60:LEU:HD12	1.93	0.51
1:A:222:VAL:HG12	1:A:330:LYS:HG2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:115:HIS:ND1	3:H:502:4EY:O2R	2.43	0.51
1:D:296:ILE:HD11	1:D:453:VAL:HG21	1.91	0.51
1:A:403:PHE:O	1:A:406:ILE:HG12	2.11	0.51
1:H:301:MET:SD	1:H:318:LEU:HB2	2.51	0.51
1:G:116:ARG:HH12	1:G:119:THR:HG23	1.76	0.51
1:G:361:TYR:O	1:G:365:GLN:HG2	2.11	0.51
1:B:210:HIS:HD2	1:B:211:HIS:ND1	2.09	0.51
1:D:226:ASN:ND2	1:D:481:PRO:O	2.43	0.51
1:F:6:GLU:HG2	1:F:302:PRO:HG3	1.93	0.51
1:C:73:ASP:OD2	3:C:502:4EY:O2R	2.27	0.51
1:B:114:LEU:HB3	1:B:401:HIS:HB2	1.91	0.51
1:C:403:PHE:O	1:C:406:ILE:HG12	2.11	0.51
1:B:296:ILE:HD11	1:B:453:VAL:HG21	1.91	0.50
1:F:322:LEU:HD13	1:F:419:ILE:HG21	1.92	0.50
1:B:282:ASN:HA	1:B:286:TYR:HD2	1.77	0.50
1:E:111:SER:HB2	1:E:200:GLY:HA3	1.93	0.50
1:C:78:GLY:H	1:C:85:ARG:NH2	2.09	0.50
1:G:31:ASP:OD2	1:G:258:THR:OG1	2.25	0.50
1:D:76:LYS:O	1:D:85:ARG:NH1	2.44	0.50
1:E:116:ARG:HH12	1:E:119:THR:HG23	1.76	0.50
1:E:320:GLN:HG2	1:E:408:CYS:HB3	1.93	0.50
1:F:364:PHE:HA	1:F:374:LEU:HD21	1.93	0.50
1:C:70:VAL:HG22	1:C:109:ILE:HB	1.93	0.50
1:G:301:MET:SD	1:G:318:LEU:HB2	2.50	0.50
1:D:226:ASN:HB3	1:D:278:TRP:HE1	1.76	0.50
1:H:241:MET:O	1:H:245:MET:HG3	2.11	0.50
1:E:75:VAL:HG12	1:E:76:LYS:HG3	1.93	0.50
1:E:111:SER:OG	1:E:196:HIS:NE2	2.44	0.50
1:E:317:MET:SD	1:E:405:MET:HG3	2.51	0.50
1:F:168:LYS:O	1:F:172:GLU:HG3	2.12	0.50
1:C:320:GLN:HG3	1:C:405:MET:HA	1.93	0.50
1:G:312:GLY:O	1:G:343:SER:OG	2.27	0.50
1:D:73:ASP:OD1	3:D:502:4EY:O2R	2.30	0.50
1:F:360:LEU:HD21	1:F:406:ILE:HD13	1.93	0.50
1:F:366:LYS:HZ2	1:F:367:GLU:HG2	1.76	0.50
1:C:32:PRO:HD2	1:C:284:ARG:HG2	1.94	0.50
1:B:356:TYR:HE2	1:B:402:GLY:HA3	1.76	0.50
1:B:437:THR:O	1:B:438:ARG:NH1	2.37	0.50
1:A:120:GLU:OE1	1:A:120:GLU:HA	2.11	0.50
1:H:51:PRO:HG3	1:H:56:PRO:HA	1.94	0.50
1:H:117:LYS:HE3	1:H:392:ARG:HA	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:360:LEU:HD21	1:E:406:ILE:HD13	1.93	0.50
1:E:401:HIS:NE2	1:E:405:MET:HE3	2.26	0.50
1:D:356:TYR:HE1	1:D:402:GLY:HA3	1.77	0.50
1:D:387:TYR:CB	1:D:399:PRO:HG3	2.42	0.50
1:H:177:ILE:HG23	1:H:250:PHE:HD2	1.76	0.50
1:F:284:ARG:HD3	1:F:284:ARG:C	2.36	0.50
1:D:190:TYR:OH	1:D:282:ASN:OD1	2.27	0.50
1:A:356:TYR:HE2	1:A:402:GLY:HA3	1.77	0.50
1:A:387:TYR:HB3	1:A:399:PRO:HG3	1.94	0.50
1:G:194:TYR:CD1	1:G:238:GLY:HA3	2.46	0.50
1:H:282:ASN:HB3	1:H:480:PRO:HB2	1.93	0.49
1:E:213:PRO:HB3	1:E:217:HIS:ND1	2.27	0.49
1:A:451:LYS:NZ	1:H:413:GLU:O	2.35	0.49
1:F:103:LYS:O	1:F:140:GLN:NE2	2.33	0.49
1:B:286:TYR:HB3	1:B:474:MET:SD	2.52	0.49
1:D:71:PHE:HB3	1:D:89:ILE:HD11	1.93	0.49
1:D:120:GLU:HA	1:D:120:GLU:OE2	2.11	0.49
1:C:257:ASP:HB3	1:C:263:ILE:HD11	1.94	0.49
1:A:238:GLY:O	1:A:242:GLU:HG2	2.12	0.49
1:B:183:GLN:HG3	1:B:256:LEU:HB2	1.94	0.49
1:A:301:MET:HE3	1:A:341:CYS:SG	2.52	0.49
1:E:226:ASN:CG	1:E:278:TRP:HE1	2.21	0.49
1:G:168:LYS:O	1:G:172:GLU:HG3	2.13	0.49
1:B:53:GLY:HA3	1:B:272:GLU:HG2	1.95	0.49
1:D:4:ASP:HB3	1:D:11:THR:HB	1.93	0.49
1:A:45:LEU:HD22	1:A:91:LEU:HD22	1.94	0.49
1:H:322:LEU:HD13	1:H:419:ILE:HG21	1.95	0.49
1:B:412:ALA:O	1:B:416:THR:OG1	2.30	0.49
1:D:226:ASN:HB3	1:D:278:TRP:NE1	2.28	0.49
1:F:116:ARG:HH12	1:F:119:THR:HG23	1.77	0.49
1:G:374:LEU:O	1:G:403:PHE:HE2	1.96	0.49
1:D:114:LEU:HB3	1:D:401:HIS:HB2	1.94	0.49
1:E:318:LEU:HD11	1:E:421:LEU:HD21	1.95	0.49
1:E:387:TYR:CB	1:E:399:PRO:HG3	2.43	0.49
1:F:192:GLY:HA2	1:F:196:HIS:HB2	1.94	0.49
1:C:387:TYR:CB	1:C:399:PRO:HG3	2.43	0.49
1:C:437:THR:O	1:C:438:ARG:NH1	2.37	0.49
1:B:194:TYR:CD1	1:B:238:GLY:HA3	2.48	0.49
1:B:257:ASP:HB3	1:B:263:ILE:HD11	1.95	0.49
1:D:319:MET:SD	1:D:435:LEU:HD21	2.52	0.49
1:A:116:ARG:NH1	1:A:122:GLU:OE1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:72:PRO:HG2	1:C:181:HIS:CD2	2.47	0.49
1:G:160:GLN:N	1:G:160:GLN:OE1	2.46	0.49
1:H:320:GLN:HG3	1:H:405:MET:HA	1.94	0.49
1:F:320:GLN:HG3	1:F:405:MET:HA	1.95	0.49
1:E:305:PHE:CD2	1:E:466:PHE:HB3	2.48	0.48
1:F:111:SER:HB2	1:F:200:GLY:HA3	1.94	0.48
1:C:178:LEU:HD11	1:C:197:CYS:HB3	1.94	0.48
1:G:177:ILE:HG23	1:G:250:PHE:HD2	1.77	0.48
1:B:406:ILE:HA	1:B:409:ALA:HB3	1.95	0.48
1:B:420:TYR:OH	1:B:447:ASP:OD2	2.27	0.48
1:C:194:TYR:CD1	1:C:238:GLY:HA3	2.48	0.48
1:C:406:ILE:HA	1:C:409:ALA:HB3	1.95	0.48
1:B:109:ILE:HD11	1:B:169:TYR:HB2	1.94	0.48
1:B:301:MET:HE3	1:B:341:CYS:SG	2.54	0.48
1:D:45:LEU:HD22	1:D:91:LEU:HD22	1.95	0.48
1:H:92:ILE:HD13	1:H:177:ILE:HG21	1.95	0.48
1:F:115:HIS:HA	1:F:397:PHE:CD2	2.49	0.48
3:F:502:4EY:O1P	3:F:502:4EY:H11	2.14	0.48
1:C:117:LYS:HE3	1:C:392:ARG:HA	1.94	0.48
1:A:10:GLY:CA	1:E:10:GLY:HA3	2.42	0.48
1:F:403:PHE:HA	1:F:406:ILE:HG12	1.96	0.48
1:G:266:ASN:HD21	1:G:276:LYS:HG2	1.78	0.48
1:B:333:MET:HG2	1:B:337:CYS:SG	2.54	0.48
1:D:194:TYR:CD1	1:D:238:GLY:HA3	2.49	0.48
1:A:387:TYR:CB	1:A:399:PRO:HG3	2.43	0.48
1:H:111:SER:HG	1:H:196:HIS:CD2	2.31	0.48
1:H:182:THR:HB	1:H:255:VAL:HG22	1.96	0.48
1:H:217:HIS:NE2	1:H:407:SER:O	2.37	0.48
1:H:302:PRO:HG2	1:H:305:PHE:HB3	1.96	0.48
1:E:232:HIS:O	1:E:236:GLU:HG3	2.14	0.48
3:E:502:4EY:O1P	3:E:502:4EY:H11	2.13	0.48
1:B:45:LEU:HD22	1:B:91:LEU:HD22	1.96	0.48
1:B:93:LEU:HD21	1:B:106:ILE:HG21	1.95	0.48
1:F:305:PHE:CD2	1:F:466:PHE:HB3	2.48	0.48
1:C:291:GLU:HG3	1:C:476:LYS:HG3	1.95	0.48
1:C:374:LEU:O	1:C:403:PHE:HE2	1.96	0.48
1:C:412:ALA:O	1:C:416:THR:OG1	2.30	0.48
1:G:305:PHE:CD2	1:G:466:PHE:HB3	2.48	0.48
1:A:216:MET:HE3	1:A:216:MET:HB2	1.74	0.48
1:E:44:THR:HG23	1:E:265:ILE:HG21	1.95	0.48
1:E:194:TYR:CD1	1:E:238:GLY:HA3	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:108:LEU:HD12	1:C:141:ILE:HG12	1.96	0.48
1:G:360:LEU:HD21	1:G:406:ILE:HD13	1.96	0.48
1:B:32:PRO:HD2	1:B:284:ARG:HG2	1.96	0.48
1:B:67:VAL:HG22	1:B:175:VAL:HB	1.95	0.48
1:B:117:LYS:HE3	1:B:392:ARG:HA	1.95	0.48
1:A:92:ILE:HD13	1:A:177:ILE:HG21	1.95	0.48
1:A:437:THR:O	1:A:438:ARG:NH1	2.38	0.48
1:F:417:ALA:HA	1:C:451:LYS:HG2	1.94	0.48
1:C:319:MET:SD	1:C:435:LEU:HD21	2.54	0.48
1:G:239:MET:O	1:G:243:GLU:HG2	2.14	0.48
1:G:317:MET:SD	1:G:405:MET:HG3	2.54	0.48
1:B:2:LYS:HA	1:B:14:ALA:O	2.14	0.48
1:B:73:ASP:OD2	3:B:502:4EY:O2R	2.31	0.48
1:B:361:TYR:O	1:B:365:GLN:HG2	2.13	0.48
1:A:51:PRO:HG3	1:A:56:PRO:HA	1.94	0.48
1:H:336:ASN:ND2	1:H:452:PHE:O	2.47	0.48
1:F:376:GLN:HB2	1:G:395:HIS:CD2	2.49	0.48
1:C:116:ARG:NH1	1:C:122:GLU:OE1	2.46	0.48
1:C:274:GLN:HG2	1:C:278:TRP:CH2	2.49	0.48
1:B:92:ILE:HD13	1:B:177:ILE:HG21	1.96	0.47
1:B:115:HIS:HA	1:B:397:PHE:CD2	2.49	0.47
3:D:502:4EY:O1P	3:D:502:4EY:H11	2.14	0.47
1:A:374:LEU:O	1:A:403:PHE:HE2	1.97	0.47
1:C:329:HIS:O	1:C:333:MET:HG3	2.14	0.47
1:B:149:TYR:HA	1:B:152:LEU:HB2	1.96	0.47
1:B:155:LEU:HD13	1:B:244:LYS:HB2	1.94	0.47
1:B:218:ARG:NE	1:B:220:ASP:OD2	2.42	0.47
1:A:70:VAL:HB	1:A:178:LEU:HD23	1.95	0.47
1:F:374:LEU:O	1:F:403:PHE:HE2	1.96	0.47
1:G:67:VAL:HG21	1:G:96:LEU:HD22	1.96	0.47
1:G:442:GLU:O	1:G:446:GLU:HG2	2.14	0.47
1:A:217:HIS:CE1	1:A:372:VAL:HG12	2.49	0.47
1:E:109:ILE:HD11	1:E:169:TYR:HB2	1.96	0.47
1:F:149:TYR:HA	1:F:152:LEU:HB2	1.96	0.47
1:F:431:ARG:NH1	1:C:368:GLY:O	2.45	0.47
1:C:116:ARG:HH12	1:C:119:THR:HG23	1.80	0.47
1:G:359:GLU:HG2	1:G:381:PHE:CZ	2.49	0.47
1:H:32:PRO:HB2	1:H:263:ILE:HG21	1.96	0.47
1:H:403:PHE:O	1:H:406:ILE:HG12	2.14	0.47
1:E:226:ASN:CB	1:E:278:TRP:HE1	2.27	0.47
1:C:223:PRO:HG3	1:C:331:ARG:HG3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:HIS:ND1	3:A:502:4EY:O2R	2.47	0.47
1:H:213:PRO:HB3	1:H:217:HIS:ND1	2.29	0.47
1:H:257:ASP:HB3	1:H:263:ILE:HD11	1.95	0.47
1:E:90:LYS:O	1:E:94:GLN:HG2	2.13	0.47
1:E:382:ALA:HB2	1:E:400:PHE:HB2	1.95	0.47
1:G:319:MET:SD	1:G:435:LEU:HD21	2.54	0.47
3:G:502:4EY:O1P	3:G:502:4EY:H11	2.14	0.47
1:D:374:LEU:O	1:D:403:PHE:HE2	1.97	0.47
1:A:166:MET:HE3	1:A:166:MET:HB2	1.81	0.47
1:A:406:ILE:HA	1:A:409:ALA:HB3	1.96	0.47
1:E:374:LEU:O	1:E:403:PHE:HE2	1.97	0.47
1:C:356:TYR:HE2	1:C:402:GLY:HA3	1.78	0.47
1:B:356:TYR:CD1	1:B:399:PRO:HA	2.50	0.47
1:D:149:TYR:HA	1:D:152:LEU:HB2	1.97	0.47
1:D:329:HIS:O	1:D:333:MET:HG3	2.15	0.47
1:A:286:TYR:HB3	1:A:474:MET:SD	2.55	0.47
1:H:194:TYR:CD1	1:H:238:GLY:HA3	2.50	0.47
1:H:374:LEU:O	1:H:403:PHE:HE2	1.98	0.47
1:E:171:TYR:HD2	1:E:245:MET:HG2	1.80	0.47
1:E:183:GLN:HG3	1:E:256:LEU:HB2	1.97	0.47
1:F:166:MET:HE2	1:F:170:VAL:HB	1.96	0.47
1:F:190:TYR:O	1:F:231:ARG:NH2	2.27	0.47
1:F:311:MET:SD	1:F:317:MET:HE3	2.54	0.47
1:F:361:TYR:O	1:F:365:GLN:HG2	2.14	0.47
1:C:71:PHE:HB3	1:C:89:ILE:HD11	1.97	0.47
1:C:314:ASN:ND2	1:C:349:PHE:O	2.43	0.47
1:C:317:MET:SD	1:C:357:LEU:HD11	2.55	0.47
1:C:419:ILE:HB	1:C:435:LEU:HD22	1.97	0.47
1:B:213:PRO:HB3	1:B:217:HIS:ND1	2.30	0.47
1:B:225:ASN:N	1:B:225:ASN:OD1	2.48	0.47
1:A:115:HIS:HA	1:A:397:PHE:CD2	2.50	0.47
1:C:115:HIS:ND1	3:C:502:4EY:O2R	2.46	0.47
1:G:232:HIS:O	1:G:236:GLU:HG3	2.15	0.47
1:D:210:HIS:HD2	1:D:211:HIS:ND1	2.13	0.47
1:D:301:MET:HG3	1:D:466:PHE:CE2	2.50	0.47
1:H:66:LYS:NZ	1:H:105:ASP:OD2	2.47	0.47
1:H:71:PHE:HB3	1:H:89:ILE:HD11	1.97	0.47
1:C:464:LYS:HB3	1:C:468:THR:HG23	1.95	0.47
1:G:166:MET:HE2	1:G:170:VAL:HB	1.97	0.47
1:B:74:ARG:H	1:B:118:ASN:HD21	1.61	0.47
1:D:324:ALA:O	1:D:328:ARG:HG3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:354:TRP:HB3	1:A:357:LEU:HG	1.97	0.47
1:H:320:GLN:HG2	1:H:408:CYS:HB3	1.96	0.47
1:H:352:SER:HB2	1:G:367:GLU:OE1	2.15	0.47
1:H:366:LYS:HB3	1:H:366:LYS:HE3	1.65	0.47
1:F:403:PHE:O	1:F:406:ILE:HG12	2.14	0.47
1:F:412:ALA:O	1:F:416:THR:OG1	2.32	0.47
1:C:62:LYS:H	1:C:65:SER:HB2	1.80	0.47
1:G:32:PRO:HB2	1:G:263:ILE:HG21	1.97	0.47
1:G:66:LYS:NZ	1:G:105:ASP:OD1	2.44	0.47
1:G:445:LEU:HG	1:G:449:LYS:HE2	1.97	0.47
1:B:354:TRP:HB3	1:B:357:LEU:HG	1.97	0.46
1:D:185:ASN:ND2	1:D:191:SER:OG	2.42	0.46
1:D:319:MET:HB3	1:D:409:ALA:HB1	1.97	0.46
1:G:71:PHE:HB3	1:G:89:ILE:HD11	1.97	0.46
1:G:356:TYR:CD2	1:G:399:PRO:HA	2.50	0.46
1:B:374:LEU:O	1:B:403:PHE:HE2	1.97	0.46
3:B:502:4EY:O1P	3:B:502:4EY:H11	2.15	0.46
1:D:108:LEU:HD12	1:D:141:ILE:HG12	1.98	0.46
1:H:87:VAL:O	1:H:91:LEU:HG	2.15	0.46
1:H:166:MET:HE2	1:H:170:VAL:HB	1.98	0.46
1:B:296:ILE:HB	1:B:459:ILE:HG12	1.97	0.46
1:D:257:ASP:HB3	1:D:263:ILE:HD11	1.98	0.46
1:A:123:ILE:HG21	1:A:141:ILE:HG21	1.96	0.46
1:A:155:LEU:HD13	1:A:244:LYS:HB2	1.97	0.46
1:A:194:TYR:CD1	1:A:238:GLY:HA3	2.50	0.46
1:A:356:TYR:CD1	1:A:399:PRO:HA	2.51	0.46
1:H:52:LEU:O	1:H:269:ALA:N	2.36	0.46
3:H:502:4EY:H11	3:H:502:4EY:O1P	2.16	0.46
1:E:149:TYR:HA	1:E:152:LEU:HB2	1.96	0.46
1:E:229:LEU:O	1:E:233:LYS:HG3	2.15	0.46
1:B:305:PHE:CD2	1:B:466:PHE:HB3	2.50	0.46
1:D:115:HIS:HA	1:D:397:PHE:CD2	2.51	0.46
1:D:178:LEU:HD11	1:D:197:CYS:HB3	1.96	0.46
1:D:354:TRP:HB3	1:D:357:LEU:HG	1.98	0.46
1:H:333:MET:HG2	1:H:337:CYS:SG	2.55	0.46
1:E:45:LEU:HD13	1:E:91:LEU:HB3	1.98	0.46
1:F:71:PHE:HB3	1:F:89:ILE:HD11	1.97	0.46
1:C:90:LYS:HZ2	1:C:90:LYS:HG2	1.49	0.46
1:G:248:LYS:HB2	1:G:248:LYS:HE3	1.82	0.46
1:G:322:LEU:HD13	1:G:419:ILE:HG21	1.97	0.46
1:B:78:GLY:O	1:B:85:ARG:NH2	2.38	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:361:TYR:O	1:D:365:GLN:HG2	2.14	0.46
1:E:387:TYR:HB3	1:E:399:PRO:HG3	1.97	0.46
1:F:213:PRO:HB3	1:F:217:HIS:ND1	2.30	0.46
1:C:356:TYR:CD1	1:C:399:PRO:HA	2.50	0.46
1:A:12:MET:HE1	1:A:423:GLY:HA3	1.98	0.46
1:F:354:TRP:HB3	1:F:357:LEU:HG	1.97	0.46
1:F:413:GLU:OE2	1:C:436:LYS:NZ	2.44	0.46
1:G:115:HIS:HA	1:G:397:PHE:CD2	2.50	0.46
1:G:271:ASP:OD1	1:G:271:ASP:N	2.44	0.46
1:G:411:LEU:HB3	1:G:415:HIS:HD2	1.80	0.46
1:A:117:LYS:HE3	1:A:392:ARG:HA	1.97	0.46
1:A:301:MET:HG2	1:A:305:PHE:CE1	2.51	0.46
1:G:87:VAL:O	1:G:91:LEU:HG	2.16	0.46
1:D:111:SER:O	1:D:111:SER:OG	2.32	0.46
1:D:216:MET:HG3	1:D:221:PHE:CE2	2.49	0.46
1:D:336:ASN:ND2	1:D:452:PHE:O	2.47	0.46
1:D:421:LEU:HD13	1:D:430:ALA:HB2	1.97	0.46
1:H:403:PHE:HA	1:H:406:ILE:HG12	1.98	0.46
1:H:406:ILE:HA	1:H:409:ALA:HB3	1.97	0.46
1:E:115:HIS:HA	1:E:397:PHE:CD2	2.51	0.46
1:B:84:HIS:O	1:B:88:SER:OG	2.30	0.46
1:B:320:GLN:HG3	1:B:405:MET:HA	1.97	0.46
1:D:212:VAL:HG22	1:D:214:LYS:H	1.80	0.46
1:A:305:PHE:CD2	1:A:466:PHE:HB3	2.50	0.46
1:A:357:LEU:HD23	1:A:357:LEU:HA	1.79	0.46
1:H:210:HIS:CE1	1:H:234:PHE:HE1	2.34	0.46
1:E:336:ASN:ND2	1:E:452:PHE:O	2.49	0.46
1:E:450:LYS:HB3	1:E:450:LYS:HE2	1.65	0.46
1:F:356:TYR:CD2	1:F:399:PRO:HA	2.51	0.46
1:C:4:ASP:HB3	1:C:11:THR:HB	1.97	0.46
1:C:51:PRO:HG3	1:C:56:PRO:HA	1.98	0.46
1:C:155:LEU:HB3	1:C:244:LYS:HG3	1.97	0.46
1:C:244:LYS:HA	1:C:244:LYS:HD2	1.82	0.46
1:G:213:PRO:HB3	1:G:217:HIS:ND1	2.30	0.46
1:B:203:HIS:O	1:B:207:ILE:HD12	2.16	0.46
1:B:402:GLY:O	1:B:405:MET:HB2	2.15	0.46
1:D:317:MET:SD	1:D:357:LEU:HD11	2.56	0.46
1:H:356:TYR:CD1	1:H:399:PRO:HA	2.51	0.46
1:C:114:LEU:HB3	1:C:401:HIS:HB2	1.97	0.46
1:G:109:ILE:HD11	1:G:169:TYR:HB2	1.98	0.46
1:B:223:PRO:HB3	1:B:330:LYS:HB3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:MET:HG3	1:A:221:PHE:CE2	2.51	0.45
1:A:322:LEU:HD13	1:A:419:ILE:HG21	1.97	0.45
3:A:502:4EY:H11	3:A:502:4EY:O1P	2.16	0.45
1:E:160:GLN:N	1:E:160:GLN:OE1	2.49	0.45
1:C:217:HIS:CE1	1:C:372:VAL:HG12	2.51	0.45
1:G:74:ARG:N	1:G:118:ASN:HD21	2.12	0.45
1:G:403:PHE:HA	1:G:406:ILE:HG12	1.97	0.45
1:B:284:ARG:NH1	1:B:471:VAL:HG12	2.30	0.45
1:D:70:VAL:HG22	1:D:109:ILE:HB	1.97	0.45
1:H:382:ALA:HB2	1:H:400:PHE:HB2	1.98	0.45
1:E:257:ASP:OD1	1:E:261:ARG:N	2.41	0.45
1:C:32:PRO:HB2	1:C:263:ILE:HG21	1.98	0.45
1:C:195:LYS:HB2	1:C:231:ARG:NH2	2.30	0.45
1:C:322:LEU:HD13	1:C:419:ILE:HG21	1.97	0.45
1:B:209:SER:OG	1:B:210:HIS:ND1	2.49	0.45
1:D:320:GLN:HG3	1:D:405:MET:HA	1.99	0.45
1:A:177:ILE:HG23	1:A:250:PHE:HD2	1.81	0.45
1:H:115:HIS:HA	1:H:397:PHE:CD2	2.51	0.45
1:H:319:MET:SD	1:H:435:LEU:HD21	2.56	0.45
1:H:356:TYR:HE2	1:H:402:GLY:HA3	1.80	0.45
1:E:23:PHE:CZ	1:E:473:LEU:HD21	2.51	0.45
1:B:216:MET:HG3	1:B:221:PHE:CE2	2.51	0.45
1:D:117:LYS:HE3	1:D:392:ARG:HA	1.98	0.45
1:A:405:MET:O	1:A:409:ALA:N	2.40	0.45
1:E:286:TYR:HB3	1:E:474:MET:SD	2.57	0.45
1:F:356:TYR:HE1	1:F:402:GLY:HA3	1.80	0.45
1:C:354:TRP:HB3	1:C:357:LEU:HG	1.99	0.45
1:D:222:VAL:HG11	1:D:415:HIS:NE2	2.31	0.45
1:D:405:MET:O	1:D:409:ALA:N	2.42	0.45
1:H:118:ASN:O	1:H:143:ASN:ND2	2.39	0.45
1:H:149:TYR:HA	1:H:152:LEU:HB2	1.98	0.45
1:E:319:MET:HE1	1:E:413:GLU:HB2	1.98	0.45
1:F:67:VAL:HG21	1:F:96:LEU:HD22	1.98	0.45
1:F:84:HIS:O	1:F:88:SER:OG	2.33	0.45
1:C:45:LEU:HD22	1:C:91:LEU:HD22	1.98	0.45
1:C:110:CYS:HB3	1:C:143:ASN:HA	1.98	0.45
1:C:343:SER:HB3	1:C:421:LEU:HD21	1.99	0.45
1:G:14:ALA:HB2	1:G:441:PHE:CD2	2.52	0.45
1:B:330:LYS:HA	1:B:330:LYS:HD2	1.80	0.45
1:D:356:TYR:CD2	1:D:399:PRO:HA	2.51	0.45
1:A:109:ILE:HD11	1:A:169:TYR:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:ARG:NE	1:A:220:ASP:OD2	2.39	0.45
1:A:317:MET:SD	1:A:357:LEU:HD11	2.57	0.45
1:E:356:TYR:CD2	1:E:399:PRO:HA	2.52	0.45
1:F:196:HIS:CD2	3:F:502:4EY:H8	2.52	0.45
1:C:108:LEU:HB2	1:C:141:ILE:HG12	1.99	0.45
1:C:301:MET:HE1	1:C:322:LEU:HG	1.98	0.45
1:D:2:LYS:HA	1:D:14:ALA:O	2.17	0.45
1:A:145:ASP:OD2	1:A:392:ARG:NE	2.43	0.45
1:A:213:PRO:HD3	1:A:407:SER:HB2	1.99	0.45
1:H:354:TRP:HB3	1:H:357:LEU:HG	1.99	0.45
1:E:226:ASN:HB3	1:E:278:TRP:CZ2	2.51	0.45
1:C:286:TYR:HB3	1:C:474:MET:SD	2.57	0.45
1:B:319:MET:HB3	1:B:409:ALA:HB1	1.98	0.45
1:A:103:LYS:NZ	1:A:140:GLN:OE1	2.50	0.45
1:A:431:ARG:NH1	1:H:368:GLY:O	2.45	0.45
1:H:445:LEU:HG	1:H:449:LYS:HE2	1.99	0.45
1:E:376:GLN:HB2	1:F:395:HIS:CD2	2.52	0.45
1:F:257:ASP:HB3	1:F:263:ILE:HD11	1.99	0.45
1:D:343:SER:HB3	1:D:421:LEU:HD21	1.99	0.45
1:D:362:ASP:O	1:D:366:LYS:HE2	2.17	0.45
1:D:368:GLY:O	1:G:431:ARG:NH1	2.44	0.45
1:A:10:GLY:HA3	1:E:10:GLY:CA	2.43	0.45
1:F:222:VAL:HG11	1:F:415:HIS:CD2	2.52	0.45
1:G:85:ARG:HE	1:G:85:ARG:HB2	1.66	0.45
1:G:193:GLY:N	1:G:253:ASP:OD2	2.48	0.45
1:G:320:GLN:HG3	1:G:405:MET:HA	1.98	0.45
1:G:387:TYR:CB	1:G:399:PRO:HG3	2.47	0.45
1:B:431:ARG:NH1	1:E:368:GLY:O	2.41	0.45
1:A:118:ASN:O	1:A:143:ASN:ND2	2.42	0.45
1:H:123:ILE:HG21	1:H:141:ILE:HG21	1.99	0.45
1:H:422:VAL:HA	1:H:438:ARG:O	2.17	0.45
1:E:301:MET:HE3	1:E:341:CYS:SG	2.57	0.45
1:E:420:TYR:CZ	1:E:436:LYS:HD3	2.52	0.45
1:C:223:PRO:HB3	1:C:330:LYS:HB3	1.99	0.45
1:G:210:HIS:CE1	1:G:234:PHE:HE1	2.34	0.45
1:G:328:ARG:HG2	1:G:472:HIS:CE1	2.52	0.45
1:B:371:LEU:HD21	1:B:433:MET:HE1	1.99	0.44
1:B:422:VAL:HA	1:B:438:ARG:O	2.18	0.44
1:D:322:LEU:HD13	1:D:419:ILE:HG21	1.98	0.44
1:A:61:ALA:HB2	1:A:175:VAL:HG21	2.00	0.44
1:F:382:ALA:HB2	1:F:400:PHE:HB2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:289:PHE:HB3	1:G:473:LEU:HD22	1.98	0.44
1:B:343:SER:HB3	1:B:421:LEU:HD21	2.00	0.44
1:B:357:LEU:HD23	1:B:357:LEU:HA	1.78	0.44
1:D:280:LEU:HD23	1:D:280:LEU:HA	1.74	0.44
1:H:281:GLY:O	1:H:285:THR:HB	2.17	0.44
1:F:114:LEU:HD22	1:F:398:HIS:CG	2.52	0.44
3:G:502:4EY:O5R	3:G:502:4EY:H1	2.17	0.44
1:B:217:HIS:CE1	1:B:372:VAL:HG12	2.53	0.44
1:B:327:ILE:HD11	1:B:411:LEU:HD23	1.99	0.44
1:D:216:MET:HE3	1:D:407:SER:OG	2.17	0.44
1:H:107:LEU:HD23	1:H:107:LEU:HA	1.86	0.44
1:H:271:ASP:OD1	1:H:271:ASP:N	2.48	0.44
1:E:311:MET:SD	1:E:317:MET:HE3	2.57	0.44
1:F:301:MET:N	1:F:342:ALA:O	2.40	0.44
1:C:422:VAL:HA	1:C:438:ARG:O	2.16	0.44
1:G:311:MET:SD	1:G:317:MET:HE3	2.58	0.44
1:G:353:LEU:HD12	1:G:353:LEU:HA	1.87	0.44
1:B:301:MET:HG2	1:B:305:PHE:CE1	2.52	0.44
1:A:351:GLU:CD	1:A:358:PRO:HG2	2.43	0.44
1:H:395:HIS:CD2	1:G:376:GLN:HB2	2.51	0.44
1:E:111:SER:O	3:E:502:4EY:O3R	2.27	0.44
1:G:178:LEU:HD12	1:G:251:CYS:SG	2.57	0.44
1:G:282:ASN:HB3	1:G:480:PRO:HB2	1.98	0.44
1:A:217:HIS:HE1	1:A:372:VAL:HG12	1.81	0.44
1:H:239:MET:O	1:H:243:GLU:HG3	2.17	0.44
1:H:475:MET:HA	1:H:475:MET:HE3	2.00	0.44
1:F:480:PRO:HA	1:F:481:PRO:HD2	1.81	0.44
1:G:418:ALA:HB1	1:G:436:LYS:HD2	2.00	0.44
1:D:115:HIS:HD1	3:D:502:4EY:H12	1.65	0.44
1:D:274:GLN:HG2	1:D:278:TRP:CH2	2.53	0.44
1:D:286:TYR:HB3	1:D:474:MET:SD	2.57	0.44
1:D:445:LEU:HD11	1:D:459:ILE:HD13	1.98	0.44
1:A:149:TYR:HA	1:A:152:LEU:HB2	1.99	0.44
1:A:183:GLN:HG2	1:A:284:ARG:NH2	2.32	0.44
1:A:320:GLN:HG3	1:A:405:MET:HA	1.99	0.44
1:C:76:LYS:O	1:C:85:ARG:NH1	2.49	0.44
1:B:37:GLU:HA	1:B:40:ILE:HD12	2.00	0.44
1:H:280:LEU:HD12	1:H:280:LEU:HA	1.78	0.44
1:E:70:VAL:HB	1:E:178:LEU:HD23	1.99	0.44
1:E:270:ALA:O	1:E:274:GLN:HG3	2.18	0.44
1:F:328:ARG:HG2	1:F:472:HIS:CD2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:115:HIS:HA	1:C:397:PHE:CD2	2.52	0.44
1:G:325:GLN:OE1	1:G:329:HIS:NE2	2.48	0.44
1:B:162:ASP:OD1	1:B:209:SER:HB2	2.17	0.44
1:B:480:PRO:HA	1:B:481:PRO:HD2	1.86	0.44
1:A:32:PRO:HD2	1:A:284:ARG:HG2	1.99	0.44
1:A:368:GLY:O	1:H:431:ARG:NH1	2.48	0.44
1:H:67:VAL:HG21	1:H:96:LEU:HD22	2.00	0.44
1:F:422:VAL:HA	1:F:438:ARG:O	2.17	0.44
1:C:210:HIS:HD2	1:C:211:HIS:ND1	2.16	0.44
1:G:192:GLY:HA2	1:G:196:HIS:HB2	2.00	0.44
1:B:51:PRO:HG3	1:B:56:PRO:HA	1.99	0.44
1:B:317:MET:SD	1:B:357:LEU:HD11	2.58	0.44
1:A:342:ALA:HB2	1:A:441:PHE:CZ	2.53	0.44
1:E:309:ASP:O	1:E:350:ASN:ND2	2.33	0.44
1:E:333:MET:HE3	1:E:337[B]:CYS:SG	2.57	0.44
1:F:213:PRO:HD3	1:F:407:SER:HB2	2.00	0.44
1:F:325:GLN:OE1	1:F:328:ARG:NH1	2.50	0.44
1:C:85:ARG:HG3	1:C:181:HIS:CE1	2.53	0.44
1:C:357:LEU:HD23	1:C:357:LEU:HA	1.79	0.44
1:C:371:LEU:HB2	1:C:410:HIS:HB2	2.00	0.44
1:D:6:GLU:HG2	1:D:467:LYS:HG3	2.00	0.43
1:D:406:ILE:HA	1:D:409:ALA:HB3	2.00	0.43
1:A:343:SER:HB3	1:A:421:LEU:HD21	2.00	0.43
1:A:422:VAL:HA	1:A:438:ARG:O	2.18	0.43
1:H:305:PHE:CG	1:H:466:PHE:HB3	2.53	0.43
1:E:226:ASN:HB3	1:E:278:TRP:HE1	1.83	0.43
1:E:354:TRP:HB3	1:E:357:LEU:HG	2.00	0.43
1:E:403:PHE:O	1:E:406:ILE:HG12	2.18	0.43
1:F:74:ARG:N	1:F:118:ASN:HD21	2.15	0.43
1:G:16:LEU:HD13	1:G:20:THR:HG21	2.00	0.43
1:G:480:PRO:HA	1:G:481:PRO:HD2	1.84	0.43
1:D:301:MET:HG2	1:D:305:PHE:CE1	2.53	0.43
1:A:116:ARG:HG2	1:A:397:PHE:CE1	2.52	0.43
1:H:70:VAL:CG1	1:H:111:SER:HB3	2.48	0.43
1:E:343:SER:HB3	1:E:421:LEU:HD21	1.99	0.43
1:F:405:MET:O	1:F:409:ALA:N	2.48	0.43
1:G:336:ASN:ND2	1:G:452:PHE:O	2.52	0.43
1:H:317:MET:SD	1:H:405:MET:HG3	2.58	0.43
1:F:301:MET:SD	1:F:318:LEU:HG	2.59	0.43
1:G:51:PRO:HG3	1:G:56:PRO:HA	1.99	0.43
1:G:354:TRP:HB3	1:G:357:LEU:HG	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:GLN:HG2	1:B:284:ARG:NH2	2.32	0.43
1:B:210:HIS:HE1	1:B:237:ILE:HD12	1.82	0.43
1:B:351:GLU:CD	1:B:358:PRO:HG2	2.43	0.43
1:D:145:ASP:OD2	1:D:392:ARG:NE	2.43	0.43
1:D:253:ASP:N	1:D:266:ASN:O	2.33	0.43
1:A:301:MET:HG3	1:A:466:PHE:CE2	2.53	0.43
1:A:420:TYR:CZ	1:A:436:LYS:HD3	2.54	0.43
1:E:271:ASP:OD1	1:E:271:ASP:N	2.50	0.43
1:F:231:ARG:HH11	1:F:278:TRP:HZ2	1.65	0.43
1:F:257:ASP:OD1	1:F:261:ARG:N	2.45	0.43
1:C:2:LYS:HA	1:C:14:ALA:O	2.18	0.43
1:C:342:ALA:HB2	1:C:441:PHE:CZ	2.54	0.43
1:C:382:ALA:HB2	1:C:400:PHE:HB2	2.00	0.43
1:A:293:LYS:HD3	1:A:293:LYS:HA	1.84	0.43
1:E:381:PHE:CG	1:E:403:PHE:HE1	2.36	0.43
1:C:213:PRO:HB3	1:C:217:HIS:CE1	2.53	0.43
1:C:301:MET:HG2	1:C:305:PHE:CE1	2.53	0.43
1:G:118:ASN:O	1:G:143:ASN:ND2	2.38	0.43
1:A:203:HIS:O	1:A:207:ILE:HD12	2.18	0.43
1:C:46:ASP:O	1:C:50:ASN:ND2	2.51	0.43
1:C:114:LEU:HD22	1:C:398:HIS:CG	2.53	0.43
1:B:301:MET:HG3	1:B:466:PHE:CE2	2.53	0.43
1:A:284:ARG:NH1	1:A:471:VAL:HG12	2.34	0.43
1:H:210:HIS:HA	1:H:215:VAL:HG11	1.99	0.43
1:H:412:ALA:O	1:H:416:THR:OG1	2.36	0.43
1:C:403:PHE:HA	1:C:406:ILE:HG12	2.00	0.43
1:H:420:TYR:CZ	1:H:436:LYS:HD3	2.54	0.43
1:E:93:LEU:HD21	1:E:106:ILE:HG21	2.01	0.43
3:E:502:4EY:O5R	3:E:502:4EY:H1	2.18	0.43
1:F:115:HIS:ND1	3:F:502:4EY:O2R	2.51	0.43
1:F:213:PRO:HB3	1:F:217:HIS:CE1	2.54	0.43
1:C:301:MET:HG3	1:C:466:PHE:CE2	2.54	0.43
1:G:171:TYR:HD2	1:G:245:MET:HG2	1.82	0.43
1:B:236:GLU:HA	1:B:239:MET:HE3	2.00	0.43
1:B:382:ALA:HB2	1:B:400:PHE:HB2	2.01	0.43
1:D:44:THR:HG23	1:D:265:ILE:HG21	2.01	0.43
1:A:22:ILE:HG12	1:A:461:ALA:HB3	1.99	0.43
1:A:403:PHE:HA	1:A:406:ILE:HG12	2.01	0.43
1:A:464:LYS:HB3	1:A:468:THR:HG23	2.00	0.43
1:H:305:PHE:CD2	1:H:466:PHE:HB3	2.53	0.43
1:E:108:LEU:HD12	1:E:141:ILE:HG12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:356:TYR:HE1	1:E:402:GLY:HA3	1.83	0.43
1:F:261:ARG:HE	1:F:261:ARG:HB2	1.73	0.43
1:F:300:GLY:HA2	1:F:342:ALA:H	1.84	0.43
1:C:213:PRO:HD3	1:C:407:SER:HB2	2.01	0.43
1:G:23:PHE:CZ	1:G:473:LEU:HD21	2.53	0.43
1:G:44:THR:HG23	1:G:265:ILE:HG21	2.01	0.43
1:B:9:HIS:CE1	1:F:344:THR:HG21	2.53	0.43
1:D:116:ARG:NH1	1:D:122:GLU:OE1	2.52	0.43
1:D:330:LYS:HD2	1:D:330:LYS:HA	1.77	0.43
1:D:402:GLY:O	1:D:405:MET:HB2	2.19	0.43
1:C:356:TYR:HA	1:C:387:TYR:CZ	2.54	0.43
1:D:22:ILE:HG12	1:D:461:ALA:HB3	2.00	0.42
1:A:213:PRO:HB3	1:A:217:HIS:CE1	2.53	0.42
1:A:412:ALA:O	1:A:416:THR:OG1	2.33	0.42
1:H:116:ARG:HH12	1:H:119:THR:HG23	1.84	0.42
1:H:257:ASP:OD1	1:H:261:ARG:N	2.46	0.42
1:H:361:TYR:O	1:H:365:GLN:HG2	2.18	0.42
1:E:14:ALA:HB2	1:E:441:PHE:CD2	2.54	0.42
1:E:166:MET:HE2	1:E:170:VAL:HB	2.00	0.42
1:E:210:HIS:CD2	1:E:234:PHE:HE1	2.37	0.42
1:E:364:PHE:HA	1:E:374:LEU:HD21	1.99	0.42
1:F:342:ALA:HB2	1:F:441:PHE:CZ	2.54	0.42
1:F:381:PHE:CG	1:F:403:PHE:HE1	2.37	0.42
1:G:256:LEU:HB3	1:G:260:SER:HA	2.01	0.42
1:B:164:VAL:HG22	1:B:237:ILE:HG23	2.01	0.42
1:E:73:ASP:OD2	3:E:502:4EY:O2R	2.37	0.42
1:E:353:LEU:HD12	1:E:353:LEU:HA	1.88	0.42
1:F:178:LEU:HD12	1:F:251:CYS:SG	2.58	0.42
1:F:194:TYR:CD1	1:F:238:GLY:HA3	2.54	0.42
1:F:196:HIS:HD2	3:F:502:4EY:H8	1.83	0.42
1:F:285:THR:O	1:F:471:VAL:HB	2.19	0.42
1:B:462:LEU:HB3	1:B:465:ALA:HB2	2.01	0.42
1:D:266:ASN:HB3	1:D:273:VAL:HG22	2.02	0.42
1:A:185:ASN:ND2	3:A:502:4EY:O2P	2.53	0.42
1:H:381:PHE:CG	1:H:403:PHE:HE1	2.37	0.42
1:F:44:THR:HG23	1:F:265:ILE:HG21	2.00	0.42
1:F:420:TYR:CZ	1:F:436:LYS:HD3	2.55	0.42
1:G:178:LEU:O	1:G:252:CYS:N	2.51	0.42
1:G:343:SER:HB3	1:G:421:LEU:HD21	2.01	0.42
1:B:182:THR:HB	1:B:255:VAL:HA	2.00	0.42
1:H:36:PRO:HD2	1:H:39:GLN:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:70:VAL:CG1	1:E:111:SER:HB3	2.49	0.42
1:C:10:GLY:CA	1:G:10:GLY:HA3	2.43	0.42
1:C:351:GLU:CD	1:C:358:PRO:HG2	2.44	0.42
1:G:331:ARG:HD2	1:G:474:MET:HG2	2.01	0.42
1:B:10:GLY:CA	1:F:10:GLY:HA3	2.43	0.42
1:D:114:LEU:N	3:D:502:4EY:O2	2.37	0.42
1:H:286:TYR:HB3	1:H:474:MET:SD	2.60	0.42
1:E:178:LEU:HD12	1:E:251:CYS:SG	2.59	0.42
1:E:319:MET:HA	1:E:322:LEU:HD12	2.00	0.42
1:F:52:LEU:O	1:F:269:ALA:N	2.39	0.42
1:D:236:GLU:HA	1:D:239:MET:HE3	2.01	0.42
1:H:111:SER:O	3:H:502:4EY:O3R	2.26	0.42
1:E:71:PHE:HB3	1:E:89:ILE:HD11	2.01	0.42
1:E:411:LEU:HD12	1:E:415:HIS:CE1	2.55	0.42
1:E:475:MET:HB2	1:E:478:ASP:CG	2.45	0.42
1:C:155:LEU:HD13	1:C:244:LYS:HB2	2.02	0.42
1:G:116:ARG:HG2	1:G:397:PHE:CE1	2.54	0.42
1:G:148:ASP:OD2	1:G:151:HIS:HD2	2.02	0.42
1:G:248:LYS:HZ2	1:G:269:ALA:HB2	1.85	0.42
1:B:10:GLY:HA3	1:F:10:GLY:CA	2.43	0.42
1:H:420:TYR:OH	1:H:447:ASP:OD2	2.32	0.42
1:G:72:PRO:HD2	1:G:85:ARG:HD3	2.01	0.42
1:H:178:LEU:HD12	1:H:251:CYS:SG	2.60	0.42
1:E:116:ARG:HG2	1:E:397:PHE:CE1	2.55	0.42
1:E:319:MET:CG	1:E:409:ALA:HB1	2.50	0.42
1:F:210:HIS:CE1	1:F:234:PHE:HE1	2.38	0.42
1:F:242:GLU:HA	1:F:245:MET:HE3	2.01	0.42
1:F:442:GLU:O	1:F:446:GLU:HG2	2.20	0.42
1:C:403:PHE:CD2	1:C:406:ILE:HD11	2.55	0.42
1:B:216:MET:HE3	1:B:216:MET:HB2	1.74	0.42
1:B:318:LEU:HD11	1:B:421:LEU:HD11	2.01	0.42
1:D:210:HIS:CD2	1:D:234:PHE:HE1	2.37	0.42
1:D:442:GLU:O	1:D:446:GLU:HG2	2.20	0.42
1:A:371:LEU:HB2	1:A:410:HIS:HB2	2.02	0.42
1:H:309:ASP:O	1:H:350:ASN:ND2	2.31	0.42
1:E:442:GLU:N	1:E:442:GLU:CD	2.78	0.42
1:F:113:GLY:O	1:F:114:LEU:HD23	2.20	0.42
1:F:224:VAL:HG12	1:F:472:HIS:CE1	2.55	0.42
1:F:251:CYS:O	1:F:267:SER:HA	2.20	0.42
1:G:420:TYR:CZ	1:G:436:LYS:HD3	2.54	0.42
1:B:442:GLU:O	1:B:446:GLU:HG2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:480:PRO:HA	1:A:481:PRO:HD2	1.88	0.42
1:E:87:VAL:O	1:E:91:LEU:HG	2.20	0.42
1:C:475:MET:HE3	1:C:475:MET:HB3	1.93	0.42
1:G:323:SER:HB3	1:G:409:ALA:HA	2.01	0.42
1:D:361:TYR:OH	1:D:429:TYR:HA	2.20	0.41
1:E:107:LEU:HD23	1:E:107:LEU:HA	1.85	0.41
1:E:269:ALA:HB3	1:E:272:GLU:HG2	2.01	0.41
1:F:90:LYS:O	1:F:94:GLN:HG2	2.19	0.41
1:F:111:SER:O	3:F:502:4EY:O3R	2.26	0.41
1:F:301:MET:HG3	1:F:466:PHE:CE2	2.55	0.41
1:C:216:MET:HE3	1:C:216:MET:HB2	1.69	0.41
1:C:371:LEU:HD21	1:C:433:MET:HE1	2.02	0.41
1:G:405:MET:HA	1:G:405:MET:HE2	2.01	0.41
1:D:53:GLY:HA3	1:D:272:GLU:HG2	2.02	0.41
1:D:301:MET:HE3	1:D:341:CYS:SG	2.60	0.41
1:H:342:ALA:HB2	1:H:441:PHE:CZ	2.56	0.41
1:H:376:GLN:HB2	1:E:395:HIS:CD2	2.55	0.41
1:E:53:GLY:HA3	1:E:272:GLU:HG3	2.01	0.41
1:E:227:ASN:O	1:E:232:HIS:NE2	2.52	0.41
1:F:443:GLU:H	1:F:443:GLU:HG3	1.63	0.41
1:C:48:ILE:HD13	1:C:92:ILE:HG13	2.03	0.41
1:C:72:PRO:HD2	1:C:85:ARG:HD3	2.03	0.41
1:H:480:PRO:HA	1:H:481:PRO:HD3	1.93	0.41
1:F:323:SER:O	1:F:327:ILE:HG13	2.20	0.41
1:D:2:LYS:HE3	1:D:2:LYS:HB3	1.73	0.41
1:H:114:LEU:HG	1:H:207:ILE:HD12	2.01	0.41
1:H:114:LEU:N	3:H:502:4EY:O2	2.34	0.41
1:H:196:HIS:CD2	3:H:502:4EY:H8	2.55	0.41
1:C:325:GLN:OE1	1:C:328:ARG:NH2	2.49	0.41
1:G:229:LEU:O	1:G:233:LYS:HG3	2.20	0.41
1:B:177:ILE:HG23	1:B:250:PHE:HD2	1.85	0.41
1:B:301:MET:HB2	1:B:341:CYS:SG	2.59	0.41
1:B:421:LEU:HD13	1:B:430:ALA:HB2	2.02	0.41
1:A:296:ILE:HB	1:A:459:ILE:HG12	2.03	0.41
1:A:353:LEU:HD12	1:A:353:LEU:HA	1.94	0.41
1:H:304:PHE:CZ	1:H:308:GLY:HA2	2.56	0.41
1:E:242:GLU:HG2	1:E:248:LYS:HA	2.02	0.41
1:F:106:ILE:O	1:F:140:GLN:NE2	2.47	0.41
1:F:309:ASP:O	1:F:350:ASN:ND2	2.34	0.41
1:D:109:ILE:HD13	1:D:142:ILE:HD11	2.01	0.41
1:A:329:HIS:O	1:A:333:MET:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:312:GLY:O	1:H:343:SER:OG	2.29	0.41
1:E:320:GLN:HG3	1:E:405:MET:HA	2.03	0.41
1:G:286:TYR:HB3	1:G:474:MET:SD	2.61	0.41
1:G:381:PHE:CG	1:G:403:PHE:HE1	2.38	0.41
1:G:406:ILE:HA	1:G:409:ALA:HB3	2.02	0.41
1:G:472:HIS:CD2	1:G:472:HIS:N	2.89	0.41
1:D:10:GLY:CA	1:H:10:GLY:HA3	2.45	0.41
1:F:445:LEU:HG	1:F:449:LYS:HE2	2.03	0.41
1:C:253:ASP:N	1:C:266:ASN:O	2.35	0.41
3:G:502:4EY:H1	3:G:502:4EY:P	2.60	0.41
1:B:158:THR:OG1	1:B:162:ASP:HB2	2.21	0.41
1:B:420:TYR:CZ	1:B:436:LYS:HD3	2.55	0.41
1:H:356:TYR:HA	1:H:387:TYR:CZ	2.56	0.41
1:C:44:THR:HG23	1:C:265:ILE:HG21	2.01	0.41
1:G:61:ALA:HB1	1:G:101:VAL:HG21	2.02	0.41
1:G:419:ILE:HB	1:G:435:LEU:HD22	2.02	0.41
1:B:158:THR:HG22	1:B:240:HIS:CG	2.56	0.41
1:B:328:ARG:HG2	1:B:472:HIS:NE2	2.35	0.41
1:D:318:LEU:HD11	1:D:421:LEU:HD11	2.02	0.41
1:D:420:TYR:CZ	1:D:436:LYS:HD3	2.55	0.41
1:D:432:GLY:O	1:G:431:ARG:NE	2.53	0.41
1:A:361:TYR:OH	1:A:429:TYR:HA	2.21	0.41
1:H:160:GLN:N	1:H:160:GLN:OE1	2.54	0.41
1:H:439:ALA:HB3	1:H:443:GLU:OE1	2.20	0.41
1:H:463:PRO:C	1:H:464:LYS:HD3	2.46	0.41
1:E:40:ILE:HD13	1:E:262:GLN:NE2	2.35	0.41
1:E:442:GLU:CD	1:E:442:GLU:H	2.29	0.41
1:F:23:PHE:CZ	1:F:473:LEU:HD21	2.56	0.41
1:F:112:ASN:O	3:F:502:4EY:H3	2.21	0.41
1:F:244:LYS:HD3	1:F:244:LYS:HA	1.90	0.41
1:F:439:ALA:HB3	1:F:443:GLU:OE1	2.21	0.41
1:G:215:VAL:HG21	1:G:233:LYS:HD2	2.01	0.41
1:G:328:ARG:HB3	1:G:472:HIS:HA	2.03	0.41
1:G:342:ALA:HB2	1:G:441:PHE:CZ	2.56	0.41
1:G:442:GLU:N	1:G:442:GLU:CD	2.79	0.41
1:B:293:LYS:HD3	1:B:293:LYS:HA	1.91	0.41
1:A:307:TYR:HB3	1:A:397:PHE:CZ	2.56	0.41
1:E:289:PHE:HB3	1:E:473:LEU:HD22	2.03	0.41
1:E:357:LEU:HD23	1:E:357:LEU:HA	1.81	0.41
1:C:336:ASN:O	1:C:336:ASN:CG	2.64	0.41
1:G:117:LYS:HE3	1:G:392:ARG:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:14:ALA:HB2	1:D:441:PHE:CD2	2.56	0.40
1:D:116:ARG:HG2	1:D:397:PHE:CE1	2.56	0.40
1:A:114:LEU:HD22	1:A:398:HIS:CG	2.56	0.40
1:A:403:PHE:CD2	1:A:406:ILE:HD11	2.56	0.40
1:A:442:GLU:O	1:A:446:GLU:HG2	2.21	0.40
1:E:251:CYS:O	1:E:267:SER:HA	2.21	0.40
1:C:301:MET:HE3	1:C:341:CYS:SG	2.61	0.40
1:D:177:ILE:HG23	1:D:250:PHE:HD2	1.86	0.40
1:A:32:PRO:HB2	1:A:263:ILE:HG21	2.03	0.40
1:E:148:ASP:OD2	1:E:151:HIS:HD2	2.04	0.40
1:F:75:VAL:HG12	1:F:76:LYS:HG3	2.02	0.40
1:F:107:LEU:HD23	1:F:107:LEU:HA	1.88	0.40
1:F:130:ASP:OD1	1:F:130:ASP:N	2.53	0.40
1:F:160:GLN:OE1	1:F:160:GLN:N	2.54	0.40
1:F:171:TYR:HD2	1:F:245:MET:HG2	1.86	0.40
1:C:216:MET:HG3	1:C:221:PHE:CE2	2.55	0.40
1:C:222:VAL:HG11	1:C:415:HIS:CE1	2.57	0.40
1:G:421:LEU:HD13	1:G:430:ALA:HB2	2.02	0.40
1:D:210:HIS:HD2	1:D:211:HIS:CE1	2.39	0.40
1:D:319:MET:HE2	1:D:433:MET:O	2.21	0.40
1:A:35:LEU:HD22	1:A:39:GLN:HG2	2.03	0.40
1:A:364:PHE:HA	1:A:374:LEU:HD11	2.04	0.40
1:H:302:PRO:HD2	1:H:305:PHE:CD1	2.56	0.40
1:E:244:LYS:HD3	1:E:244:LYS:HA	1.82	0.40
1:F:195:LYS:HZ2	3:F:502:4EY:H4	1.65	0.40
1:C:210:HIS:CD2	1:C:234:PHE:HE1	2.39	0.40
1:C:305:PHE:CD2	1:C:466:PHE:HB3	2.57	0.40
1:G:225:ASN:OD1	1:G:225:ASN:N	2.54	0.40
1:G:382:ALA:HB2	1:G:400:PHE:HB2	2.03	0.40
1:H:251:CYS:O	1:H:267:SER:HA	2.22	0.40
1:E:118:ASN:O	1:E:143:ASN:ND2	2.41	0.40
1:C:183:GLN:HG2	1:C:256:LEU:HB2	2.04	0.40
1:C:296:ILE:HB	1:C:459:ILE:HG12	2.02	0.40
1:C:361:TYR:OH	1:C:429:TYR:HA	2.21	0.40
1:G:403:PHE:CD2	1:G:406:ILE:HD11	2.56	0.40
1:G:476:LYS:HB3	1:G:476:LYS:HE3	1.75	0.40
1:B:51:PRO:HG2	1:B:54:MET:O	2.22	0.40
1:B:231:ARG:NH1	1:B:274:GLN:OE1	2.54	0.40
1:D:356:TYR:HA	1:D:387:TYR:CZ	2.57	0.40
1:D:395:HIS:CD2	1:A:376:GLN:HB2	2.56	0.40
1:E:248:LYS:HB3	1:E:248:LYS:HE2	1.79	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:463:PRO:C	1:E:464:LYS:HD3	2.46	0.40
1:C:226:ASN:HB3	1:C:278:TRP:HE1	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	479/498 (96%)	471 (98%)	8 (2%)	0	100	100
1	B	478/498 (96%)	469 (98%)	9 (2%)	0	100	100
1	C	479/498 (96%)	466 (97%)	13 (3%)	0	100	100
1	D	479/498 (96%)	472 (98%)	7 (2%)	0	100	100
1	E	479/498 (96%)	468 (98%)	11 (2%)	0	100	100
1	F	478/498 (96%)	469 (98%)	9 (2%)	0	100	100
1	G	479/498 (96%)	467 (98%)	12 (2%)	0	100	100
1	H	478/498 (96%)	467 (98%)	11 (2%)	0	100	100
All	All	3829/3984 (96%)	3749 (98%)	80 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	400/425 (94%)	395 (99%)	5 (1%)	61	76
1	B	398/425 (94%)	394 (99%)	4 (1%)	68	81
1	C	400/425 (94%)	395 (99%)	5 (1%)	61	76
1	D	400/425 (94%)	394 (98%)	6 (2%)	57	73
1	E	402/425 (95%)	398 (99%)	4 (1%)	68	81
1	F	402/425 (95%)	398 (99%)	4 (1%)	68	81
1	G	402/425 (95%)	398 (99%)	4 (1%)	68	81
1	H	402/425 (95%)	399 (99%)	3 (1%)	76	87
All	All	3206/3400 (94%)	3171 (99%)	35 (1%)	63	79

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	224	VAL
1	B	243	GLU
1	B	335	ASP
1	B	411	LEU
1	D	210	HIS
1	D	216	MET
1	D	224	VAL
1	D	278	TRP
1	D	411	LEU
1	D	471	VAL
1	A	207	ILE
1	A	224	VAL
1	A	278	TRP
1	A	374	LEU
1	A	471	VAL
1	H	66	LYS
1	H	126	VAL
1	H	215	VAL
1	E	66	LYS
1	E	126	VAL
1	E	262	GLN
1	E	411	LEU
1	F	126	VAL
1	F	130	ASP
1	F	411	LEU
1	F	421	LEU
1	C	65	SER

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Mol	Chain	Res	Type
1	C	111	SER
1	C	224	VAL
1	C	278	TRP
1	C	336	ASN
1	G	66	LYS
1	G	207	ILE
1	G	262	GLN
1	G	471	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	9	HIS
1	B	39	GLN
1	B	50	ASN
1	B	84	HIS
1	B	160	GLN
1	B	336	ASN
1	B	376	GLN
1	B	415	HIS
1	B	455	GLN
1	D	185	ASN
1	D	196	HIS
1	D	210	HIS
1	D	266	ASN
1	D	274	GLN
1	A	376	GLN
1	A	401	HIS
1	A	410	HIS
1	A	415	HIS
1	H	134	GLN
1	H	240	HIS
1	H	262	GLN
1	H	376	GLN
1	H	410	HIS
1	H	415	HIS
1	E	210	HIS
1	E	410	HIS
1	F	262	GLN
1	F	274	GLN
1	F	376	GLN
1	F	415	HIS

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Mol	Chain	Res	Type
1	C	183	GLN
1	C	210	HIS
1	C	401	HIS
1	C	410	HIS
1	C	455	GLN
1	G	151	HIS
1	G	226	ASN
1	G	376	GLN
1	G	410	HIS
1	G	415	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	4EY	F	502	2,1	22,25,25	3.33	8 (36%)	27,37,37	1.56	3 (11%)
3	4EY	E	502	2,1	22,25,25	3.32	8 (36%)	27,37,37	1.52	3 (11%)
3	4EY	G	502	2,1	22,25,25	3.33	8 (36%)	27,37,37	1.49	3 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	4EY	H	502	2,1	22,25,25	3.33	8 (36%)	27,37,37	1.54	3 (11%)
3	4EY	A	502	2,1	22,25,25	3.31	8 (36%)	27,37,37	1.53	3 (11%)
3	4EY	C	502	2,1	22,25,25	3.31	8 (36%)	27,37,37	1.60	3 (11%)
3	4EY	D	502	2,1	22,25,25	3.32	8 (36%)	27,37,37	1.59	3 (11%)
3	4EY	B	502	2,1	22,25,25	3.32	8 (36%)	27,37,37	1.55	3 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	4EY	F	502	2,1	-	3/12/32/32	0/2/2/2
3	4EY	E	502	2,1	-	3/12/32/32	0/2/2/2
3	4EY	G	502	2,1	-	3/12/32/32	0/2/2/2
3	4EY	H	502	2,1	-	3/12/32/32	0/2/2/2
3	4EY	A	502	2,1	-	3/12/32/32	0/2/2/2
3	4EY	C	502	2,1	-	3/12/32/32	0/2/2/2
3	4EY	D	502	2,1	-	3/12/32/32	0/2/2/2
3	4EY	B	502	2,1	-	3/12/32/32	0/2/2/2

All (64) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	502	4EY	O4R-C1R	9.98	1.54	1.40
3	H	502	4EY	O4R-C1R	9.98	1.54	1.40
3	G	502	4EY	O4R-C1R	9.97	1.54	1.40
3	C	502	4EY	O4R-C1R	9.96	1.54	1.40
3	A	502	4EY	O4R-C1R	9.94	1.53	1.40
3	E	502	4EY	O4R-C1R	9.94	1.53	1.40
3	B	502	4EY	O4R-C1R	9.94	1.53	1.40
3	D	502	4EY	O4R-C1R	9.93	1.53	1.40
3	F	502	4EY	C3R-C4R	-7.19	1.34	1.53
3	E	502	4EY	C3R-C4R	-7.19	1.34	1.53
3	H	502	4EY	C3R-C4R	-7.16	1.34	1.53
3	G	502	4EY	C3R-C4R	-7.16	1.34	1.53
3	B	502	4EY	C3R-C4R	-7.15	1.34	1.53
3	D	502	4EY	C3R-C4R	-7.12	1.34	1.53
3	A	502	4EY	C3R-C4R	-7.12	1.34	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	502	4EY	C3R-C4R	-7.12	1.34	1.53
3	H	502	4EY	O4R-C4R	6.81	1.60	1.45
3	D	502	4EY	O4R-C4R	6.79	1.60	1.45
3	F	502	4EY	O4R-C4R	6.79	1.60	1.45
3	B	502	4EY	O4R-C4R	6.78	1.60	1.45
3	E	502	4EY	O4R-C4R	6.75	1.60	1.45
3	A	502	4EY	O4R-C4R	6.74	1.60	1.45
3	C	502	4EY	O4R-C4R	6.74	1.60	1.45
3	G	502	4EY	O4R-C4R	6.73	1.59	1.45
3	G	502	4EY	C2R-C3R	3.09	1.61	1.53
3	F	502	4EY	C4-C5	-3.08	1.34	1.39
3	D	502	4EY	C2R-C3R	3.06	1.61	1.53
3	B	502	4EY	C2R-C3R	3.05	1.61	1.53
3	E	502	4EY	C2R-C3R	3.05	1.61	1.53
3	C	502	4EY	C2R-C3R	3.05	1.61	1.53
3	A	502	4EY	C2R-C3R	3.03	1.61	1.53
3	H	502	4EY	C2R-C3R	3.02	1.61	1.53
3	F	502	4EY	C2R-C3R	3.02	1.61	1.53
3	H	502	4EY	C4-C5	-2.99	1.35	1.39
3	E	502	4EY	C4-C5	-2.98	1.35	1.39
3	D	502	4EY	C4-C5	-2.96	1.35	1.39
3	G	502	4EY	C4-C5	-2.95	1.35	1.39
3	G	502	4EY	C4-C3	-2.94	1.34	1.39
3	F	502	4EY	C4-C3	-2.94	1.34	1.39
3	D	502	4EY	C4-C3	-2.93	1.34	1.39
3	B	502	4EY	C4-C5	-2.93	1.35	1.39
3	E	502	4EY	C4-C3	-2.92	1.34	1.39
3	C	502	4EY	C4-C5	-2.90	1.35	1.39
3	C	502	4EY	C4-C3	-2.89	1.34	1.39
3	H	502	4EY	C4-C3	-2.89	1.34	1.39
3	A	502	4EY	C4-C5	-2.88	1.35	1.39
3	A	502	4EY	C4-C3	-2.87	1.34	1.39
3	B	502	4EY	C4-C3	-2.85	1.34	1.39
3	D	502	4EY	C1-S2	2.29	1.82	1.74
3	G	502	4EY	C1-S2	2.29	1.82	1.74
3	C	502	4EY	C1-S2	2.28	1.82	1.74
3	F	502	4EY	C1-S2	2.28	1.82	1.74
3	A	502	4EY	C1-S2	2.28	1.82	1.74
3	H	502	4EY	C1-S2	2.27	1.82	1.74
3	B	502	4EY	C1-S2	2.27	1.82	1.74
3	E	502	4EY	C1-S2	2.24	1.82	1.74
3	E	502	4EY	C3-C7	2.18	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	502	4EY	C3-C7	2.18	1.54	1.46
3	F	502	4EY	C3-C7	2.17	1.54	1.46
3	A	502	4EY	C3-C7	2.17	1.54	1.46
3	H	502	4EY	C3-C7	2.17	1.54	1.46
3	B	502	4EY	C3-C7	2.15	1.54	1.46
3	C	502	4EY	C3-C7	2.14	1.54	1.46
3	D	502	4EY	C3-C7	2.12	1.54	1.46

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	502	4EY	C4R-O4R-C1R	-5.90	104.52	109.92
3	H	502	4EY	C4R-O4R-C1R	-5.85	104.57	109.92
3	F	502	4EY	C4R-O4R-C1R	-5.69	104.71	109.92
3	B	502	4EY	C4R-O4R-C1R	-5.69	104.72	109.92
3	E	502	4EY	C4R-O4R-C1R	-5.68	104.73	109.92
3	D	502	4EY	C4R-O4R-C1R	-5.61	104.79	109.92
3	A	502	4EY	C4R-O4R-C1R	-5.56	104.83	109.92
3	G	502	4EY	C4R-O4R-C1R	-5.46	104.92	109.92
3	C	502	4EY	C3-C2-N1	-2.73	118.96	121.28
3	D	502	4EY	C2-C3-C4	2.65	120.27	117.52
3	C	502	4EY	C2-C3-C4	2.61	120.23	117.52
3	B	502	4EY	C2-C3-C4	2.48	120.09	117.52
3	A	502	4EY	C2-C3-C4	2.48	120.09	117.52
3	D	502	4EY	C3-C2-N1	-2.48	119.17	121.28
3	A	502	4EY	C3-C2-N1	-2.43	119.21	121.28
3	F	502	4EY	C2-C3-C4	2.42	120.03	117.52
3	H	502	4EY	C3-C2-N1	-2.39	119.25	121.28
3	F	502	4EY	C3-C2-N1	-2.37	119.26	121.28
3	E	502	4EY	C3-C2-N1	-2.36	119.27	121.28
3	B	502	4EY	C3-C2-N1	-2.35	119.28	121.28
3	G	502	4EY	C2-C3-C4	2.33	119.93	117.52
3	H	502	4EY	C2-C3-C4	2.32	119.93	117.52
3	E	502	4EY	C2-C3-C4	2.32	119.93	117.52
3	G	502	4EY	C3-C2-N1	-2.30	119.33	121.28

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	502	4EY	C5R-O5R-P-O2P
3	B	502	4EY	O4R-C4R-C5R-O5R

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Mol	Chain	Res	Type	Atoms
3	D	502	4EY	O4R-C4R-C5R-O5R
3	A	502	4EY	O4R-C4R-C5R-O5R
3	H	502	4EY	O4R-C4R-C5R-O5R
3	F	502	4EY	O4R-C4R-C5R-O5R
3	C	502	4EY	C5R-O5R-P-O2P
3	C	502	4EY	O4R-C4R-C5R-O5R
3	G	502	4EY	C5R-O5R-P-O2P
3	E	502	4EY	O4R-C4R-C5R-O5R
3	G	502	4EY	O4R-C4R-C5R-O5R
3	D	502	4EY	C3R-C4R-C5R-O5R
3	H	502	4EY	C3R-C4R-C5R-O5R
3	F	502	4EY	C3R-C4R-C5R-O5R
3	A	502	4EY	C3R-C4R-C5R-O5R
3	E	502	4EY	C3R-C4R-C5R-O5R
3	B	502	4EY	C3R-C4R-C5R-O5R
3	C	502	4EY	C3R-C4R-C5R-O5R
3	G	502	4EY	C3R-C4R-C5R-O5R
3	D	502	4EY	C5R-O5R-P-O2P
3	A	502	4EY	C5R-O5R-P-O2P
3	H	502	4EY	C5R-O5R-P-O2P
3	E	502	4EY	C5R-O5R-P-O2P
3	F	502	4EY	C5R-O5R-P-O2P

There are no ring outliers.

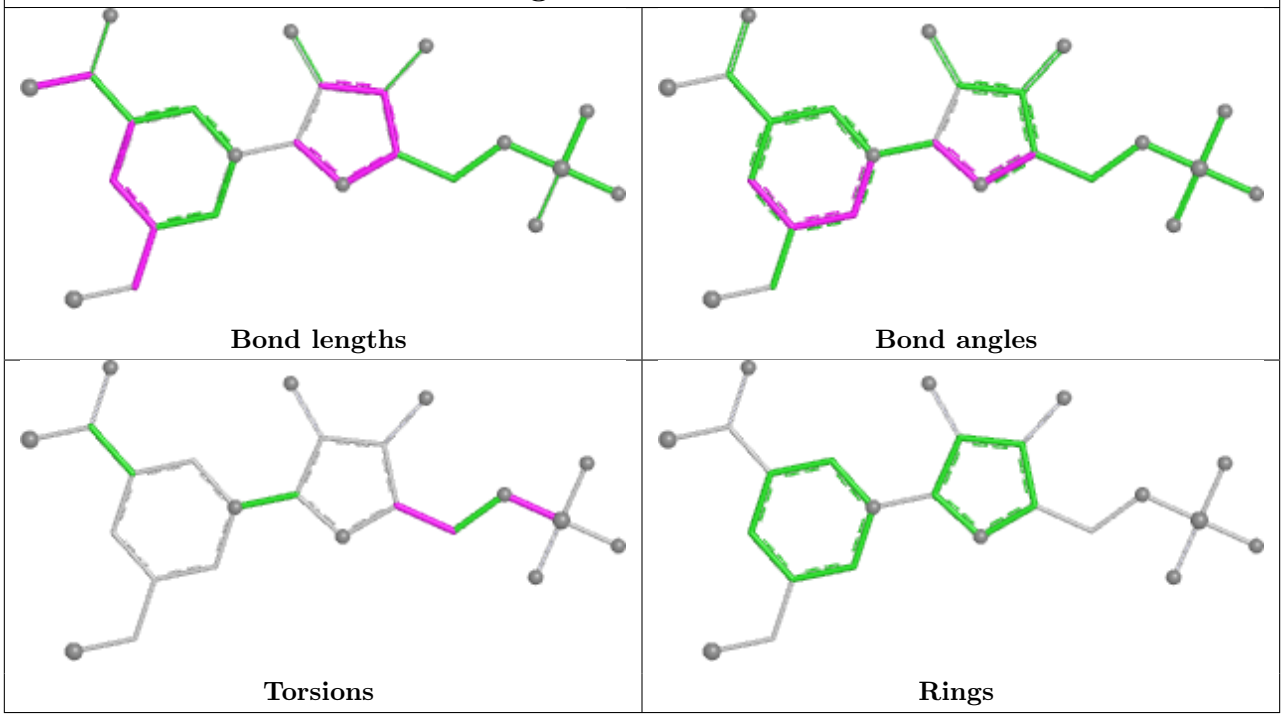
8 monomers are involved in 40 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	502	4EY	7	0
3	E	502	4EY	5	0
3	G	502	4EY	5	0
3	H	502	4EY	6	0
3	A	502	4EY	4	0
3	C	502	4EY	5	0
3	D	502	4EY	5	0
3	B	502	4EY	3	0

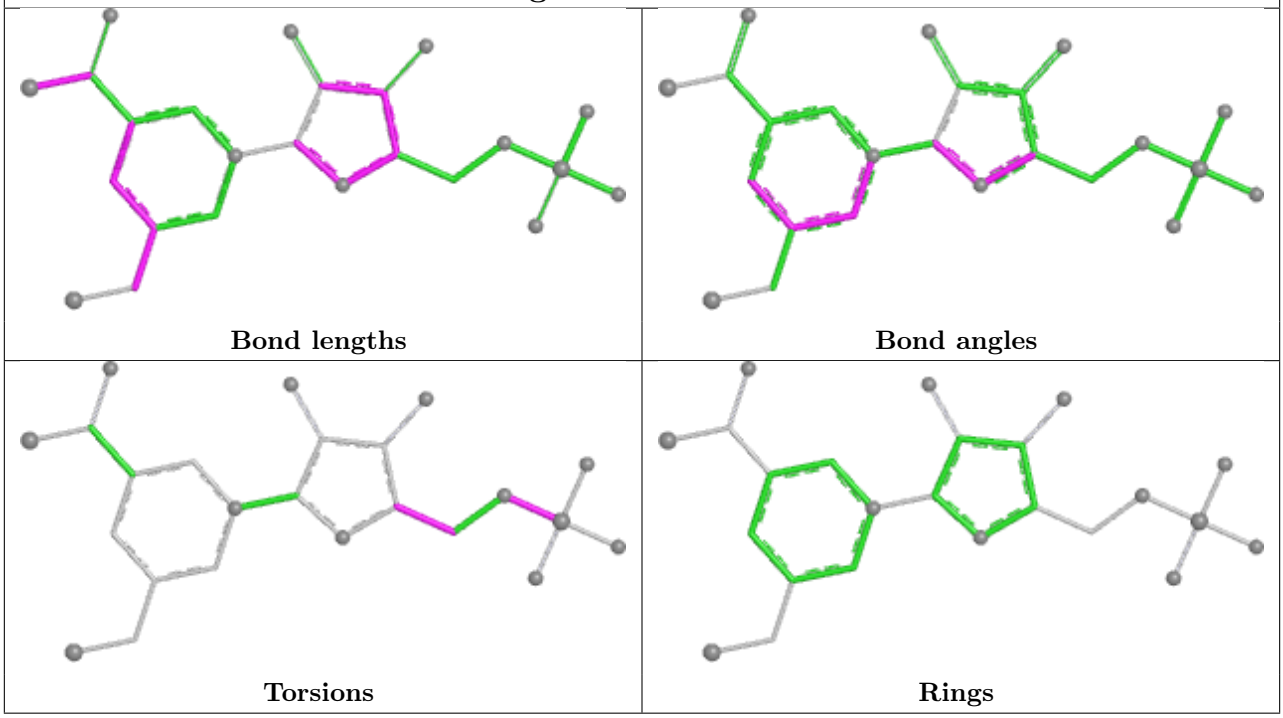
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

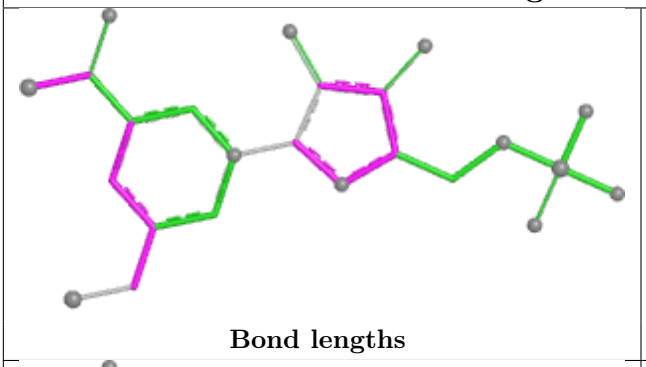
Ligand 4EY F 502



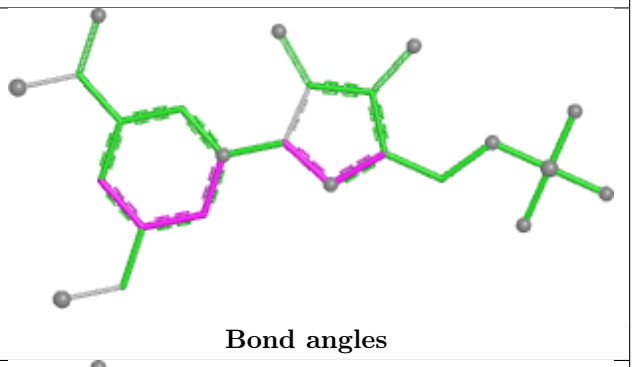
Ligand 4EY E 502



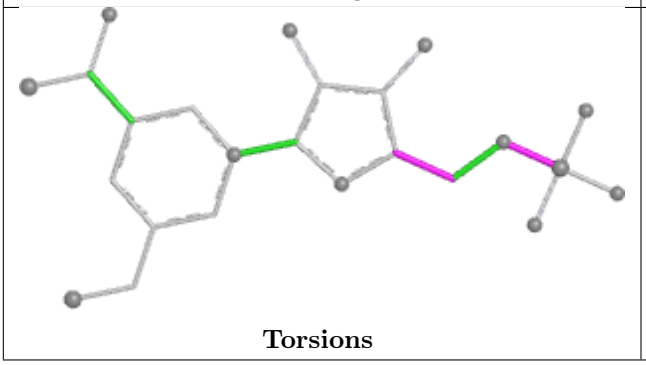
Ligand 4EY G 502



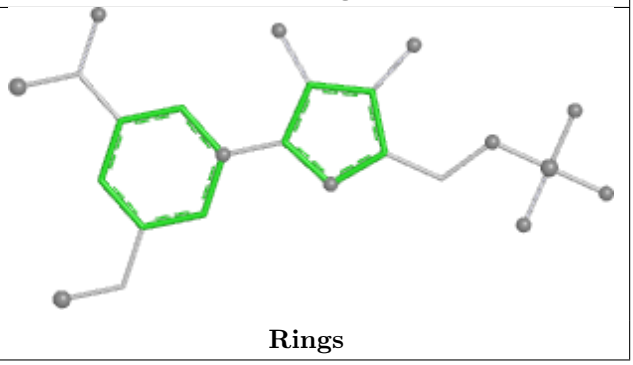
Bond lengths



Bond angles

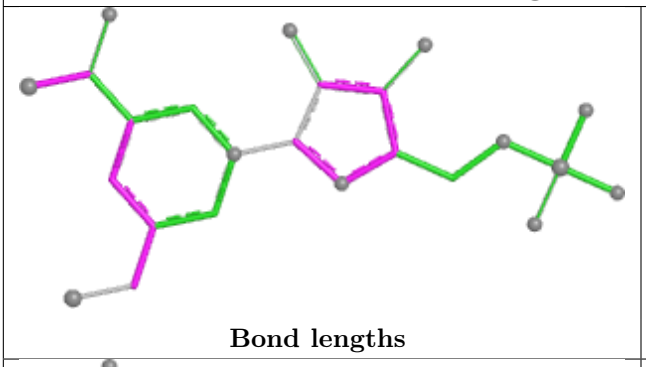


Torsions

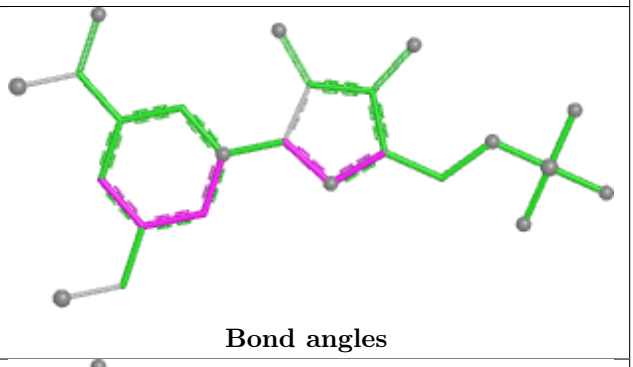


Rings

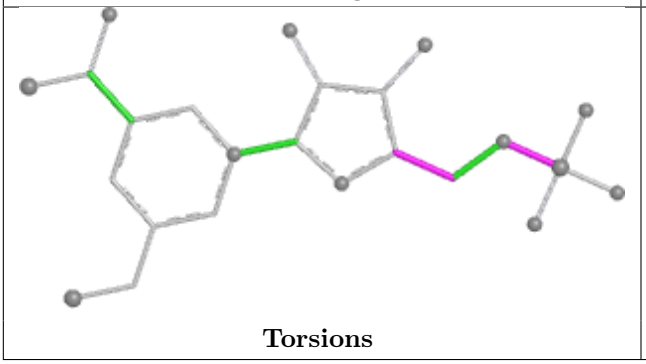
Ligand 4EY H 502



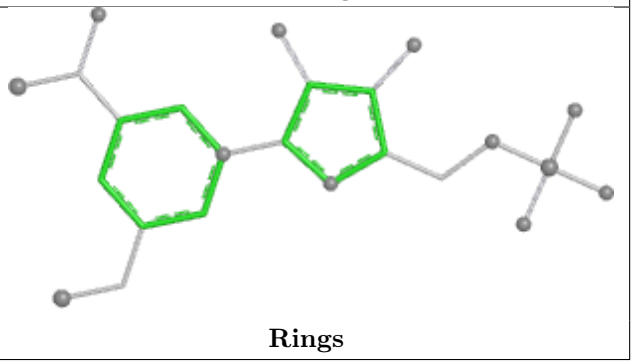
Bond lengths



Bond angles

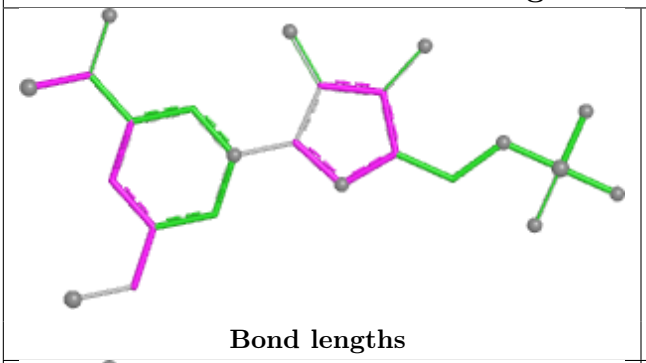


Torsions

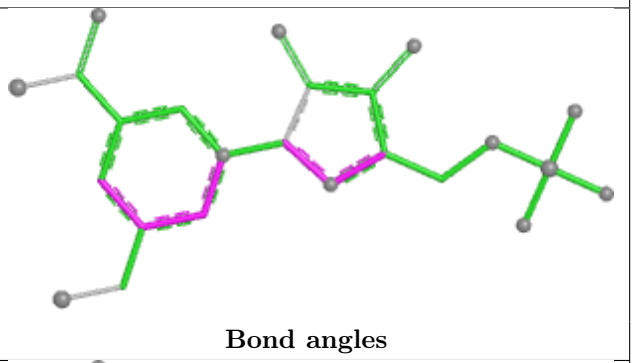


Rings

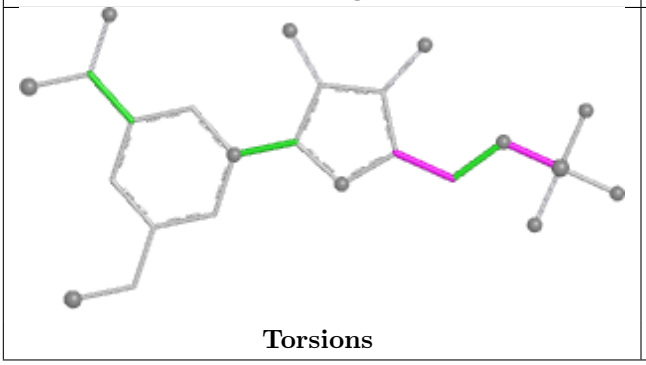
Ligand 4EY A 502



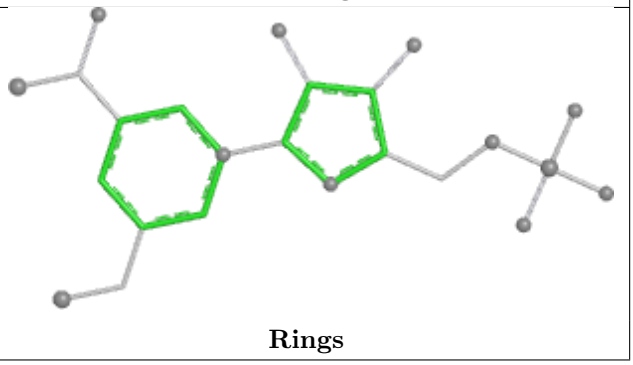
Bond lengths



Bond angles

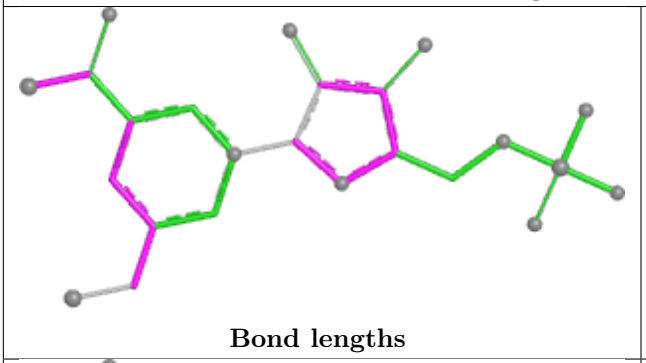


Torsions

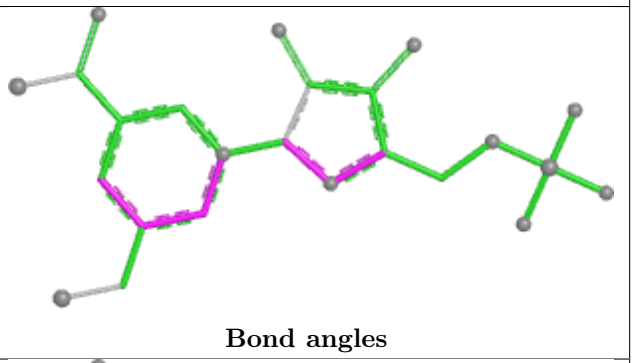


Rings

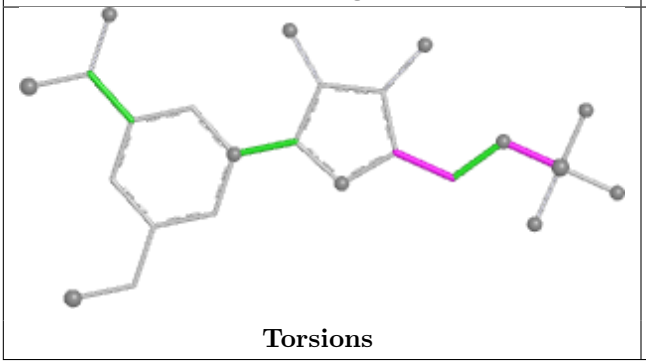
Ligand 4EY C 502



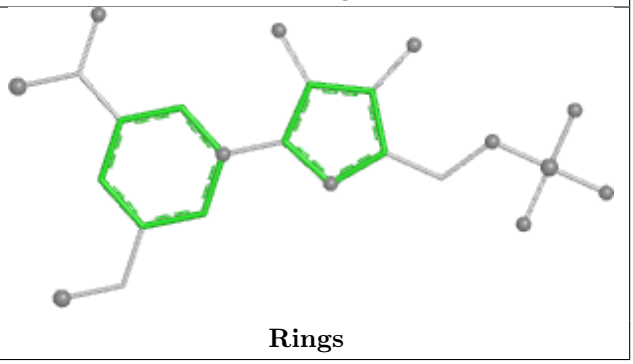
Bond lengths



Bond angles

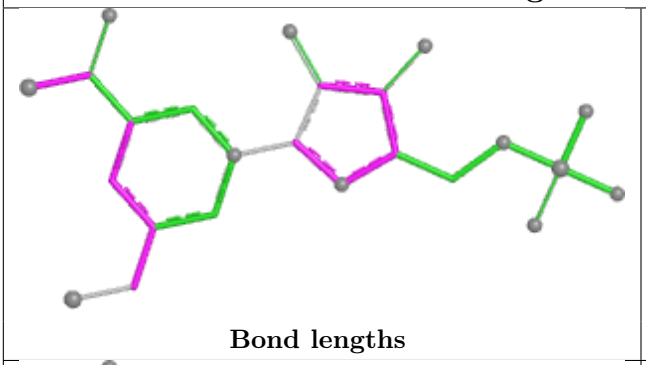


Torsions

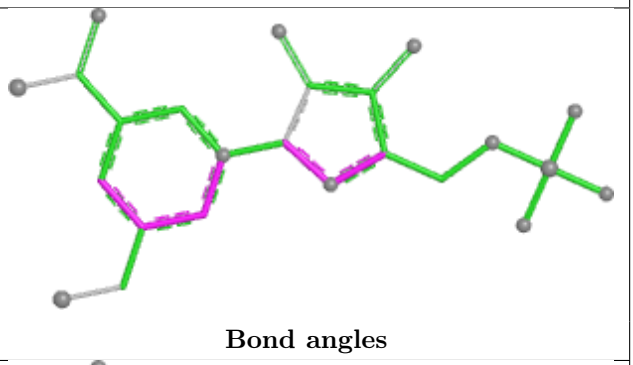


Rings

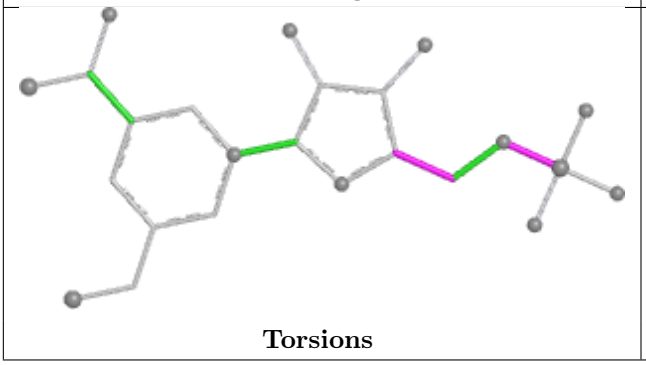
Ligand 4EY D 502



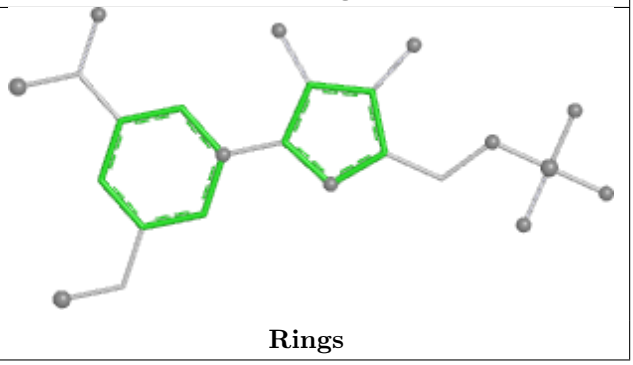
Bond lengths



Bond angles

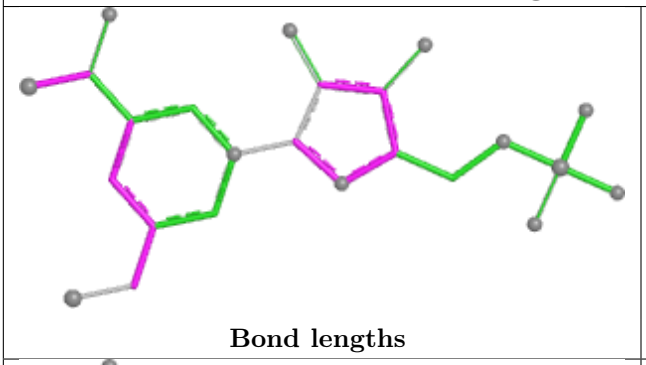


Torsions

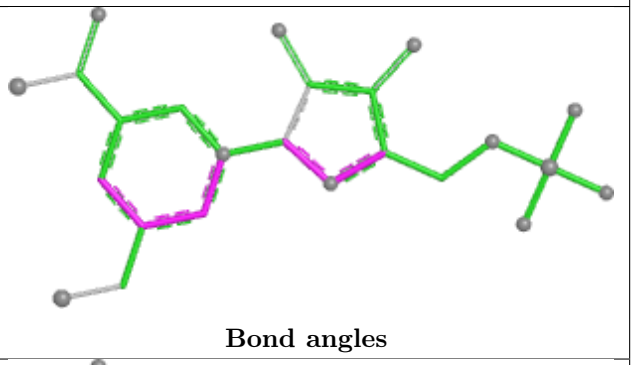


Rings

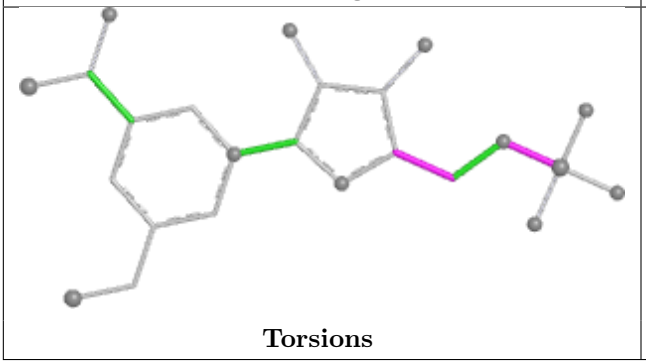
Ligand 4EY B 502



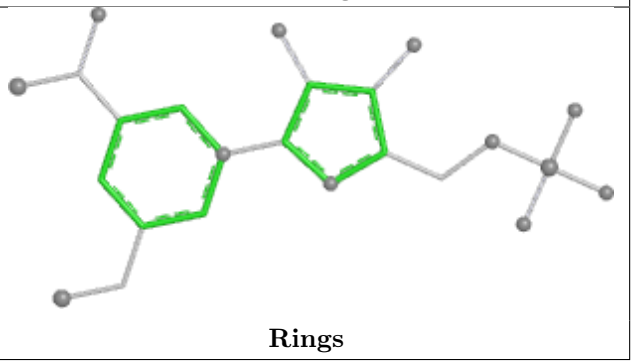
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

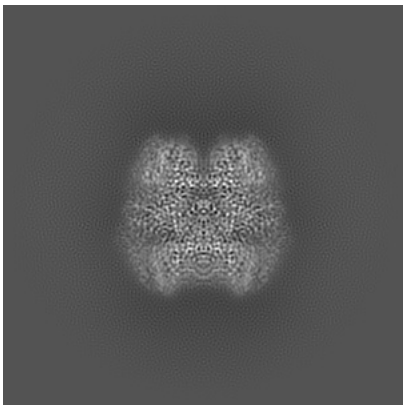
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-72200. These allow visual inspection of the internal detail of the map and identification of artifacts.

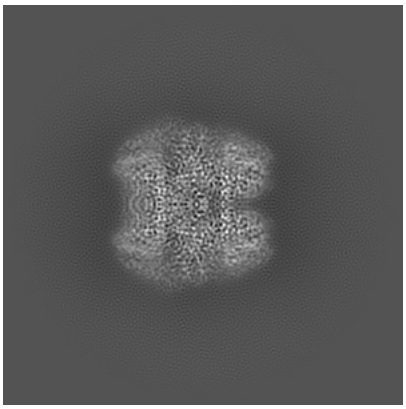
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

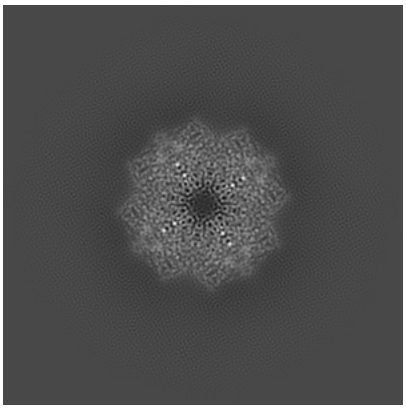
6.1.1 Primary map



X

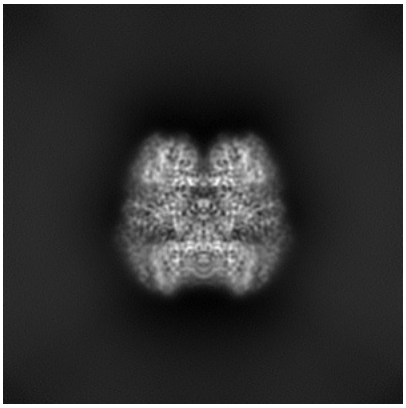


Y

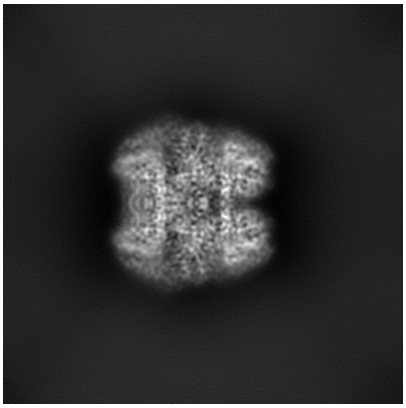


Z

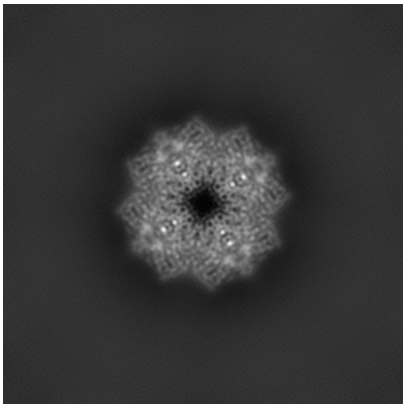
6.1.2 Raw map



X



Y

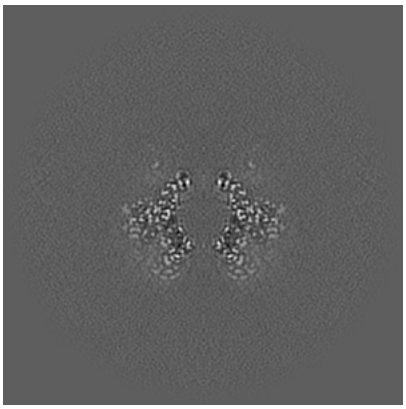


Z

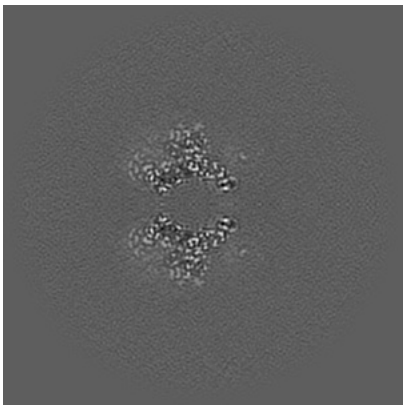
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

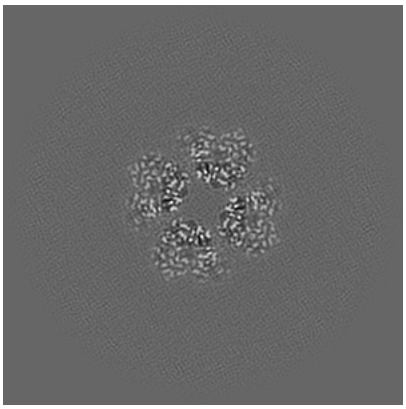
6.2.1 Primary map



X Index: 150

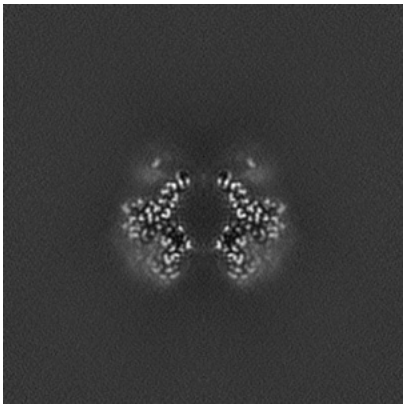


Y Index: 150

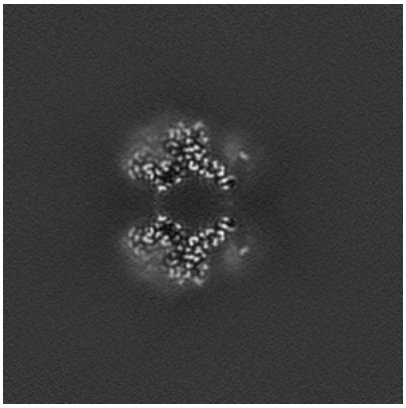


Z Index: 150

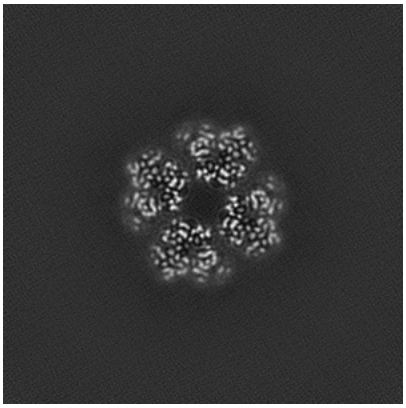
6.2.2 Raw map



X Index: 150



Y Index: 150

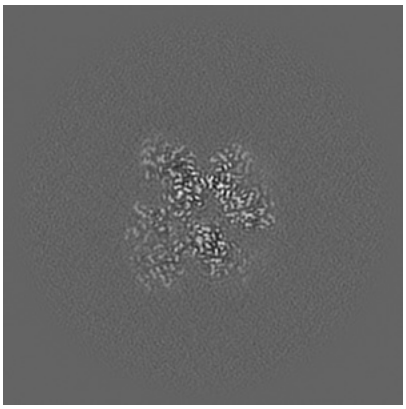


Z Index: 150

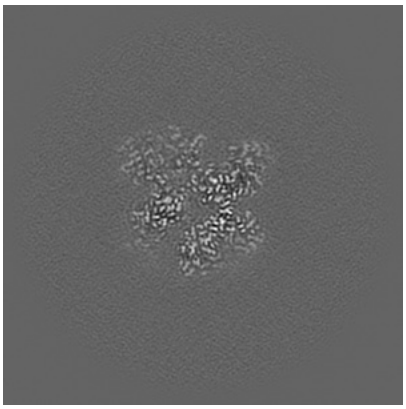
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

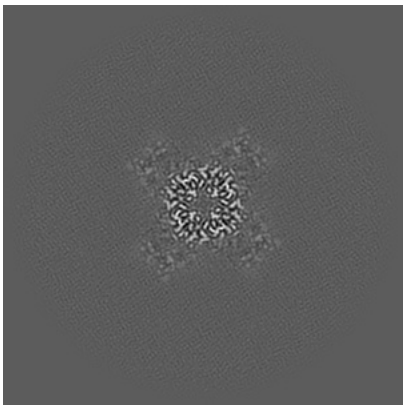
6.3.1 Primary map



X Index: 168

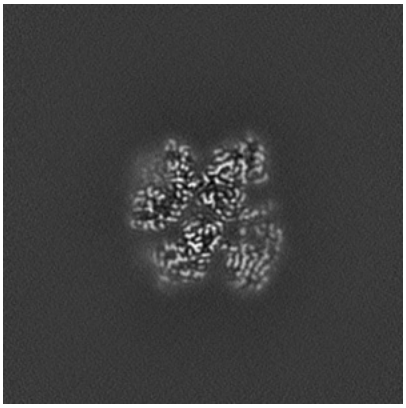


Y Index: 168

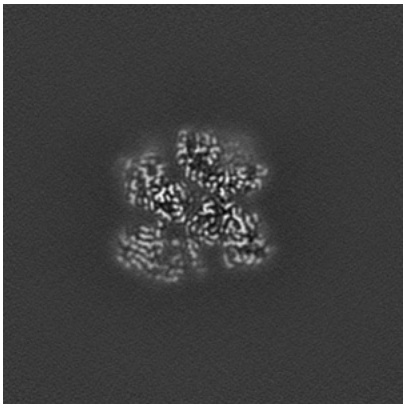


Z Index: 164

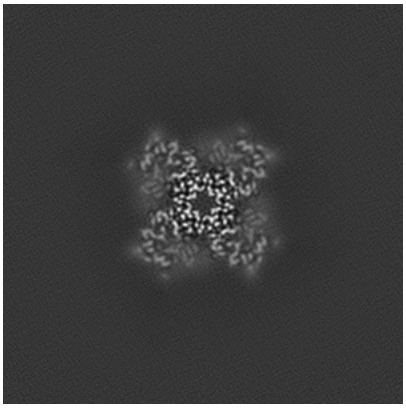
6.3.2 Raw map



X Index: 130



Y Index: 130

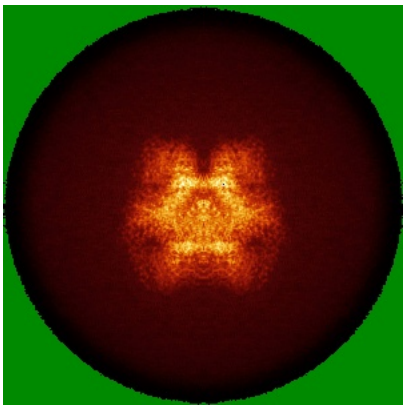


Z Index: 167

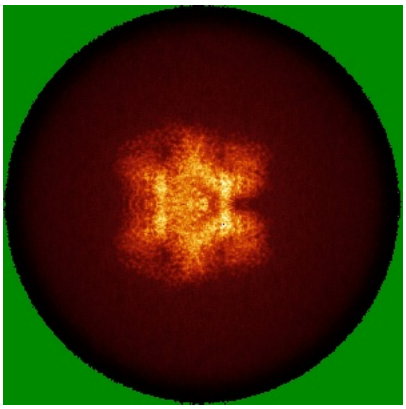
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

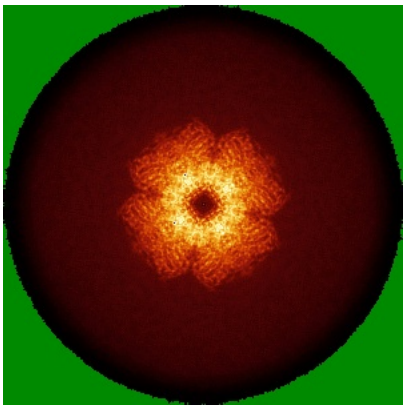
6.4.1 Primary map



X

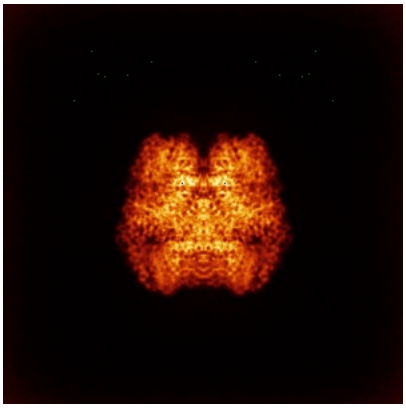


Y

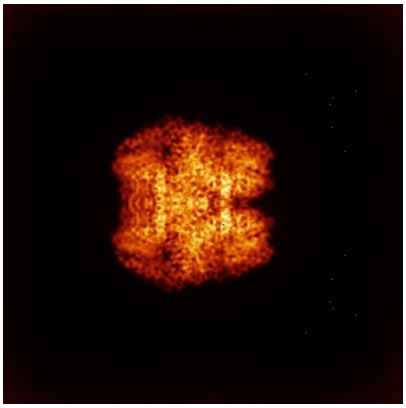


Z

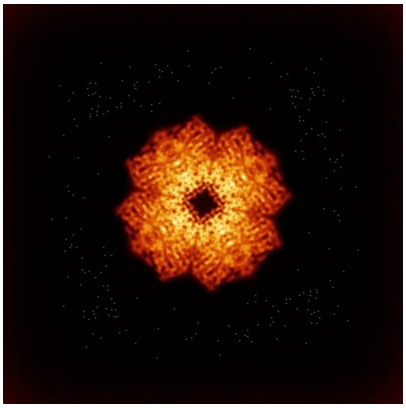
6.4.2 Raw map



X



Y

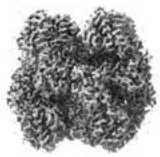


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.11. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X

Y

Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

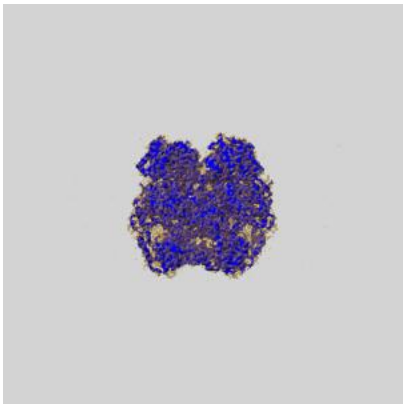
6.6 Mask visualisation

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

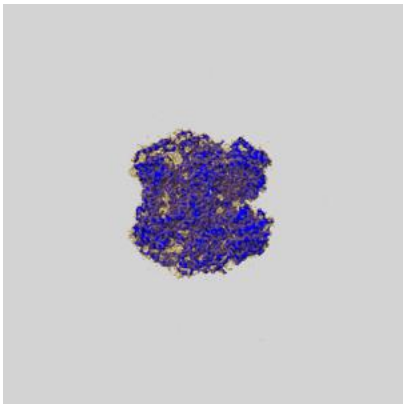
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

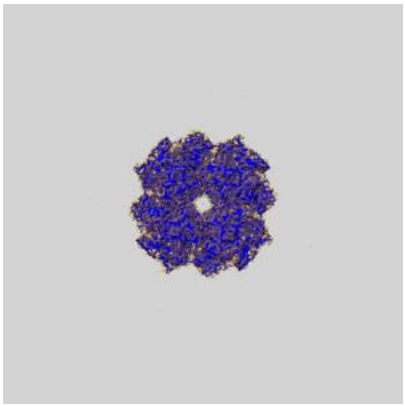
6.6.1 emd_72200_msk_1.map



X



Y

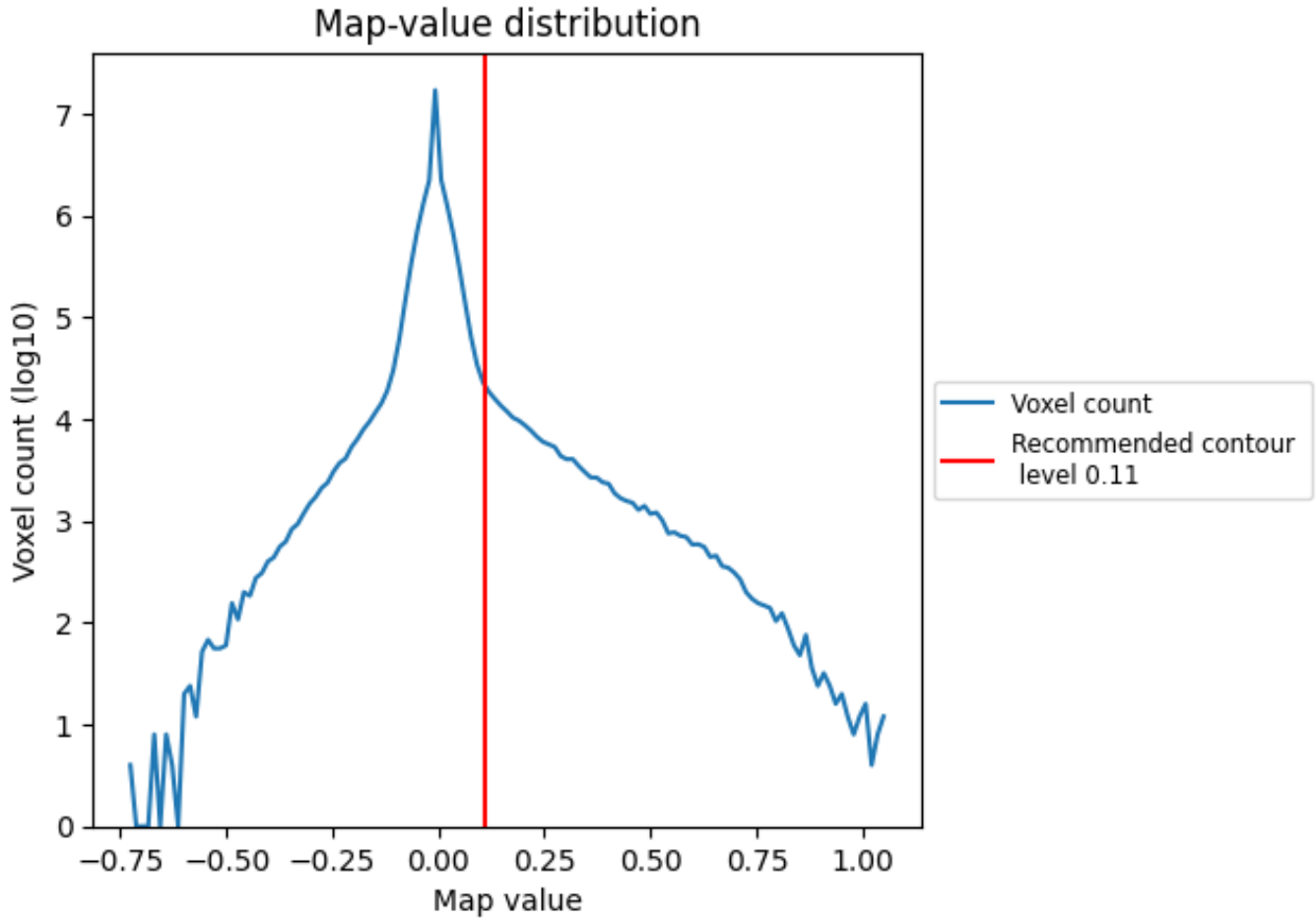


Z

7 Map analysis

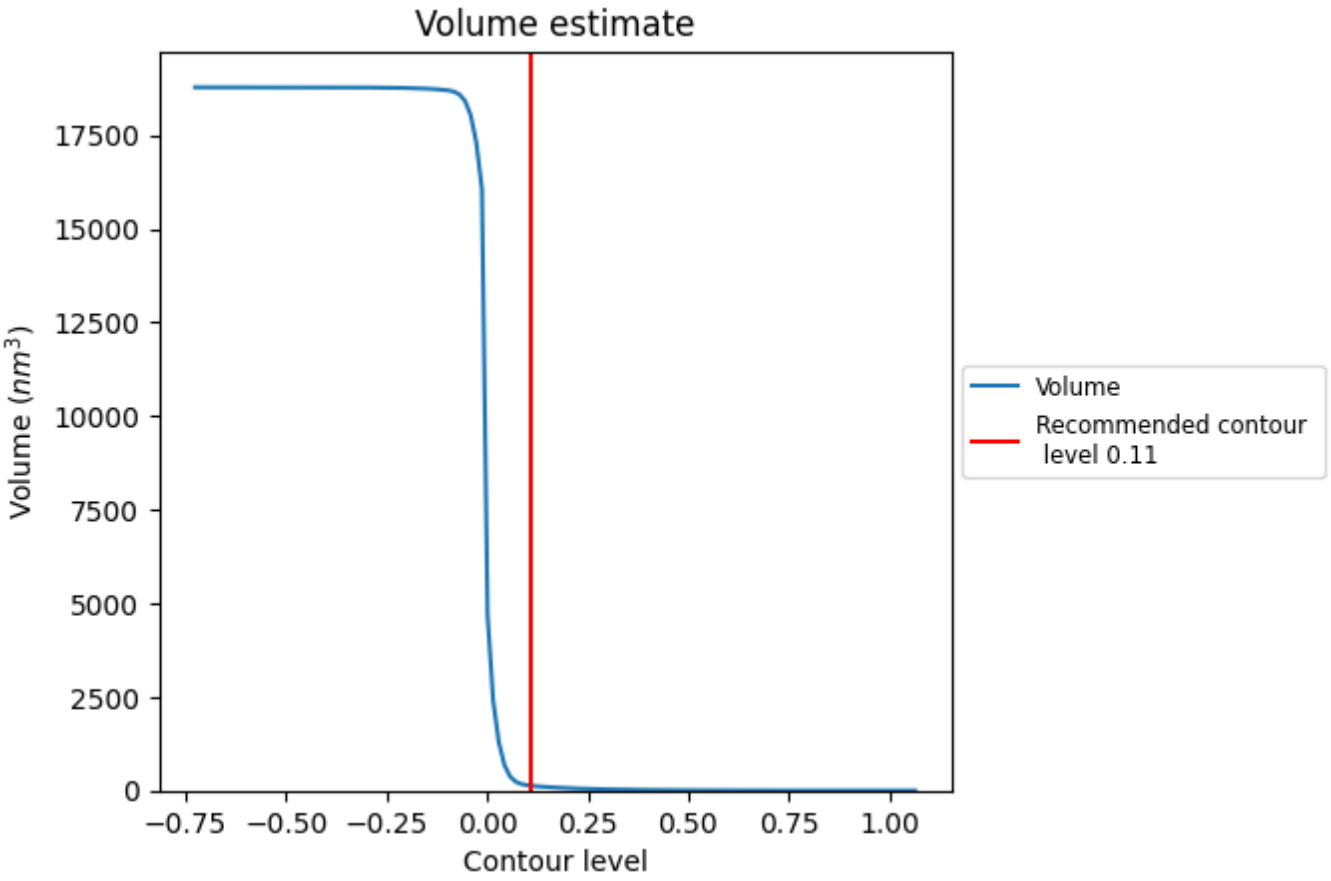
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

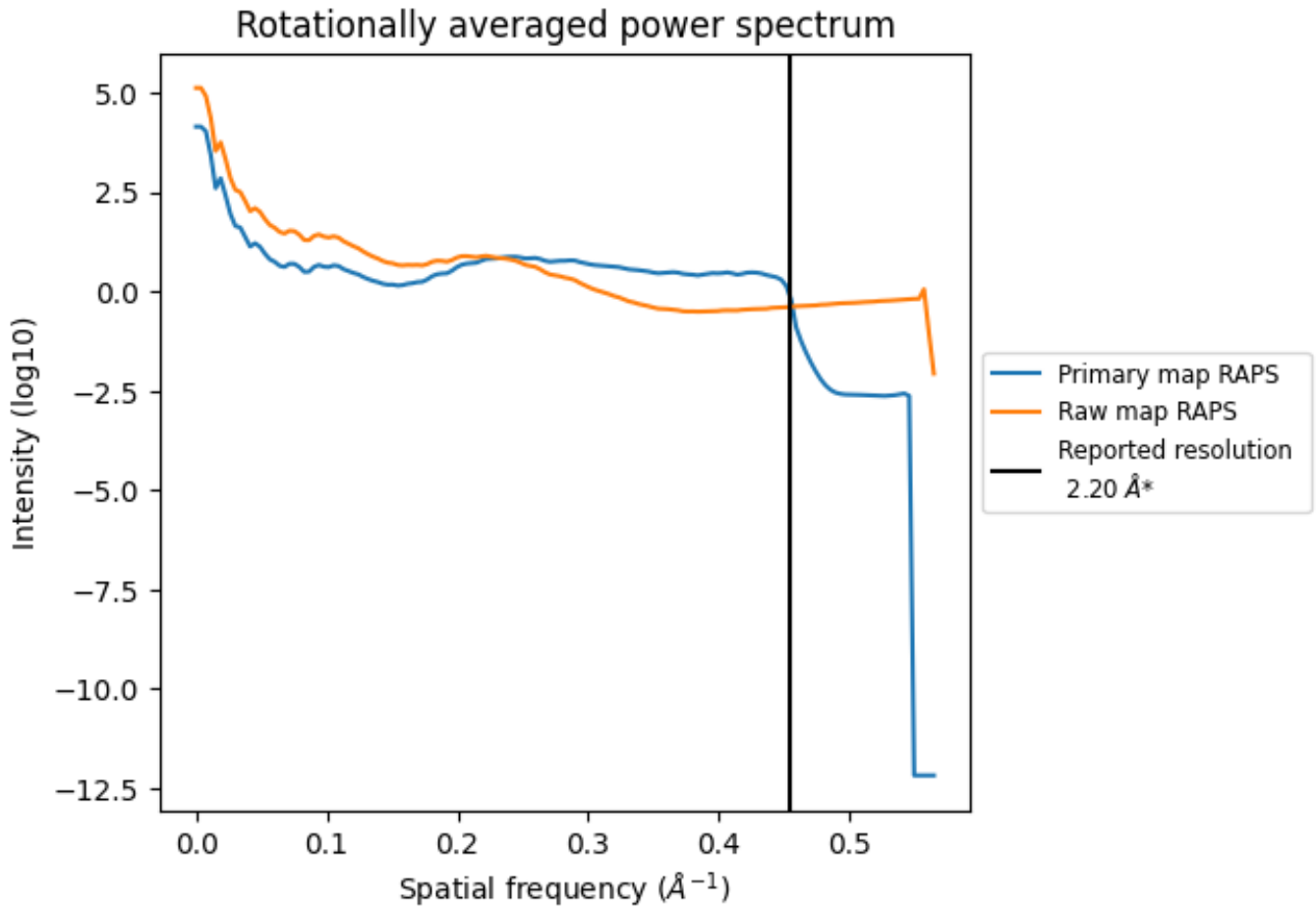
7.2 Volume estimate



The volume at the recommended contour level is 129 nm^3; this corresponds to an approximate mass of 117 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

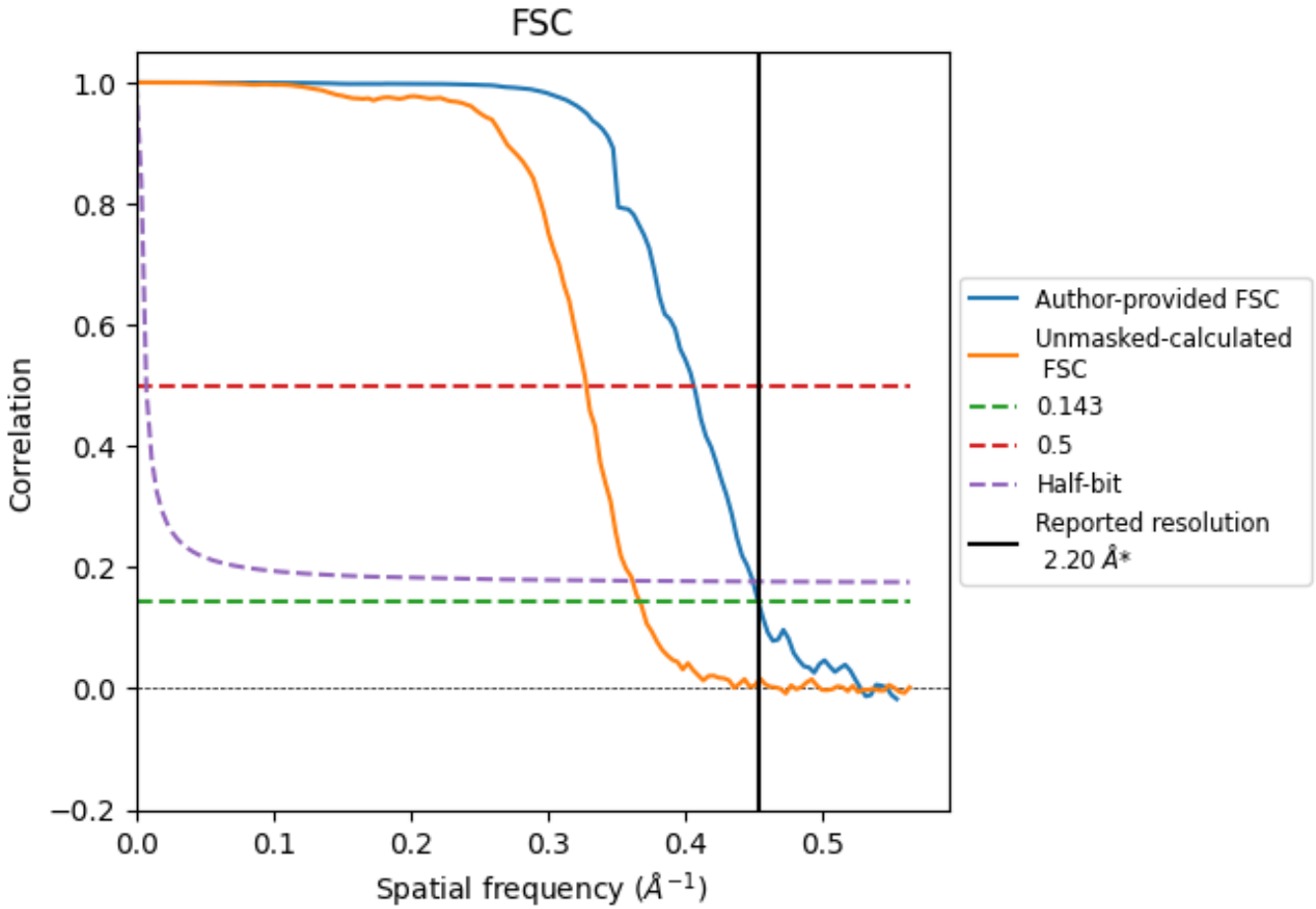


*Reported resolution corresponds to spatial frequency of 0.455 $Å^{-1}$

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.455 Å^{-1}

8.2 Resolution estimates (i)

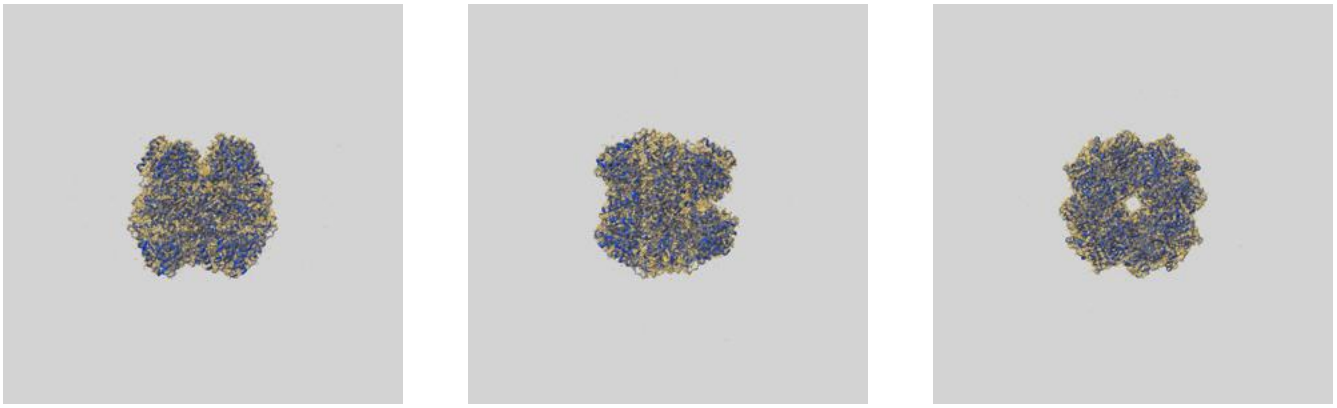
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.20	-	-
Author-provided FSC curve	2.20	2.46	2.22
Unmasked-calculated*	2.72	3.05	2.76

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.72 differs from the reported value 2.2 by more than 10 %

9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-72200 and PDB model 9Q3K. Per-residue inclusion information can be found in section 3 on page 6.

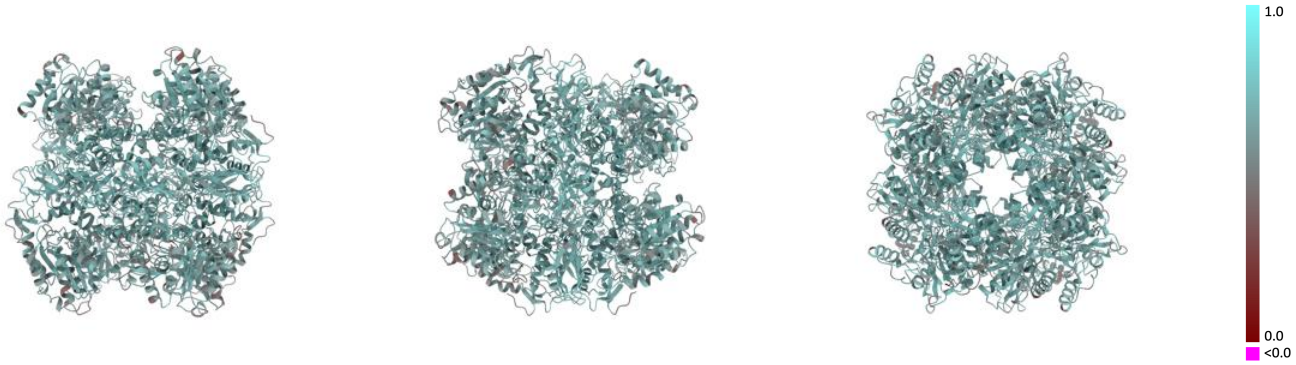
9.1 Map-model overlay



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.11 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

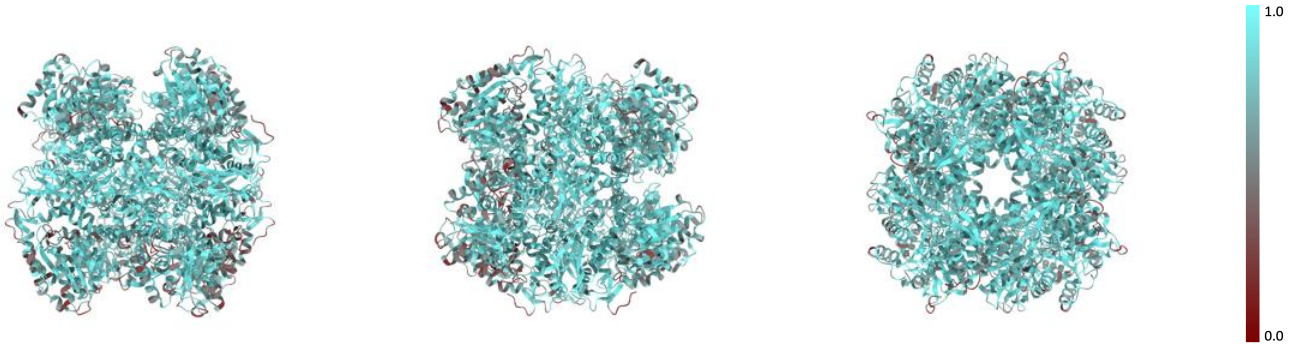
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

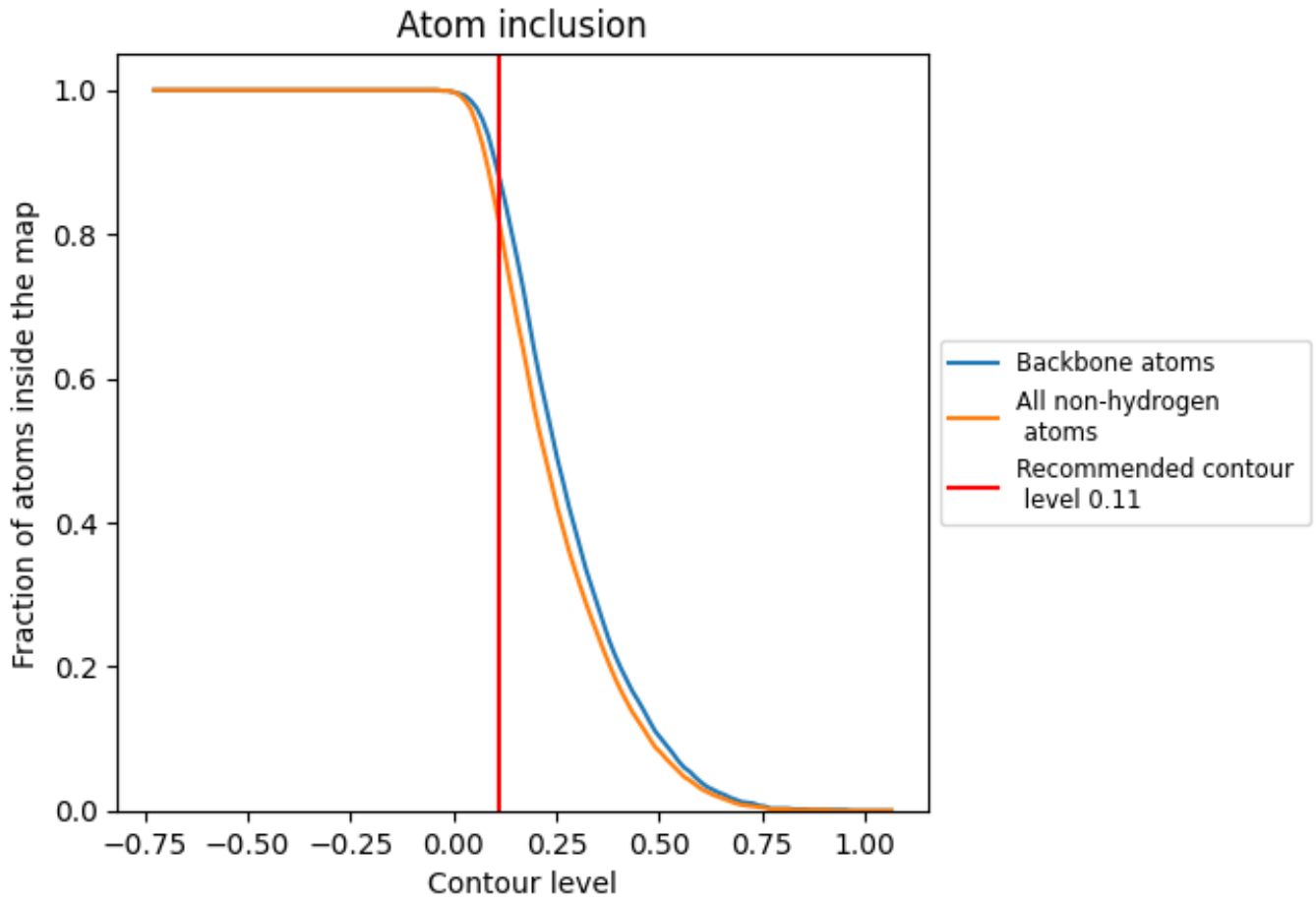
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.11).

9.4 Atom inclusion (i)



At the recommended contour level, 88% of all backbone atoms, 82% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.11) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8200	0.6490
A	0.7990	0.6420
B	0.8040	0.6450
C	0.7980	0.6390
D	0.7990	0.6420
E	0.8390	0.6540
F	0.8420	0.6560
G	0.8390	0.6550
H	0.8380	0.6570